QUANTUM SPIN Doctors Dissect Exotic States of MATTER

At the cutting edge of condensed matter research, scientists are using several resources to investigate extraordinary states of matter. With over a million processor hours provided by a DOE INCITE grant, researchers are working on simulations that shed light on two unfamiliar quantum phases, Bose–Einstein condensation and Bose glass. To physically demonstrate these phases, the team is collaborating with investigators at the National High Magnetic Field Laboratory at Los Alamos National Laboratory.

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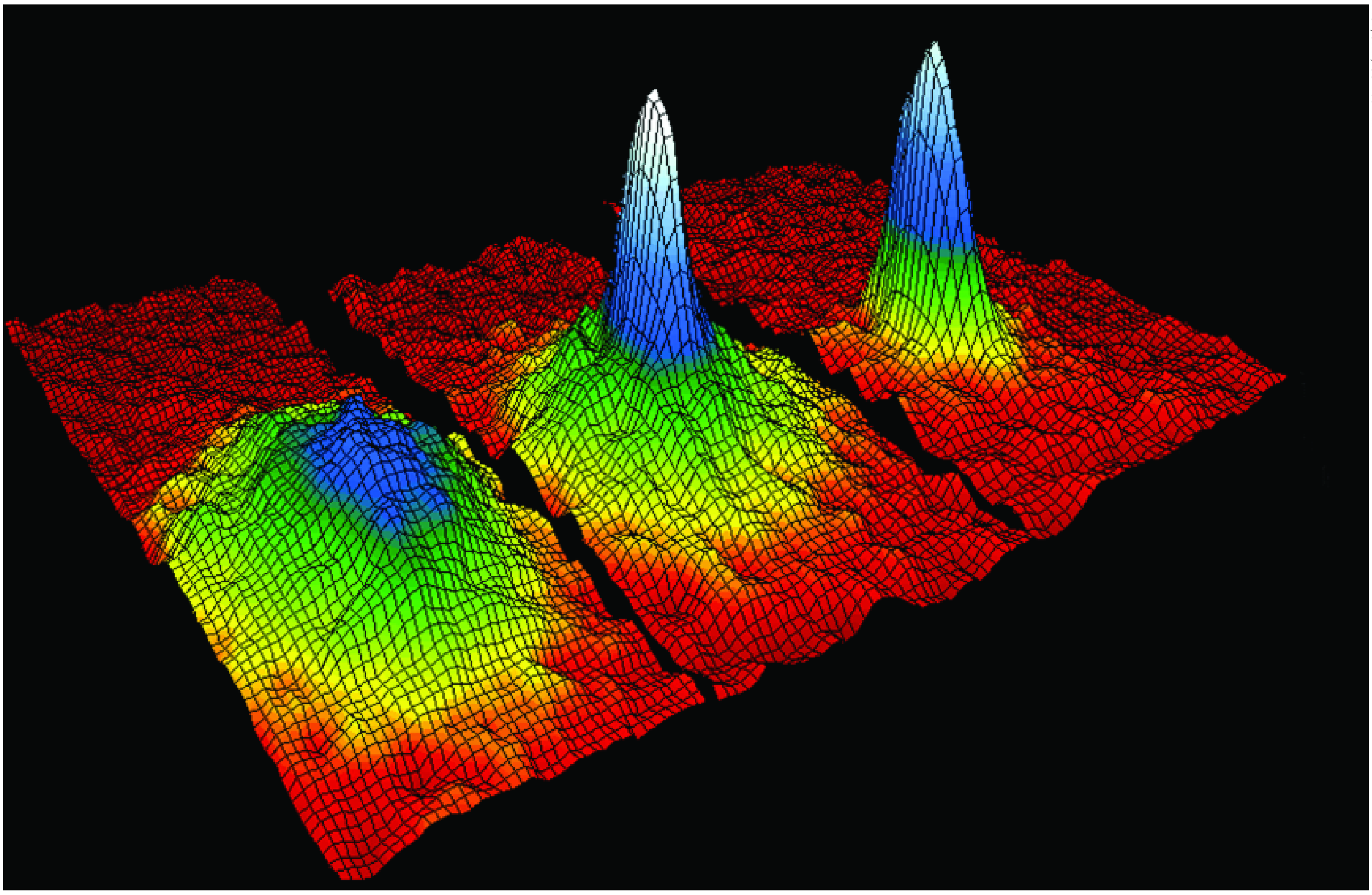
When German physicist Max Planck became the father of quantum theory in 1900, he was not trying to revolutionize the world. He did not envision microchips, flash memory, or the myriad accomplishments that allow a dual-core processor with 230 million transistors to fit in the laptop computer you carry under your arm.

Planck had a much more modest and immediate need, namely to provide a theoretical foundation for the way in which a heated object such as a light bulb radiates energy. The classical physics of the day predicted incorrectly that the heated object would radiate energy primarily at high frequencies and short wavelengths, emitting copious ultraviolet rays and X-rays. In fact, however, the dominant frequency emitted by the object changed depending on its temperature.

In response to this conundrum, known hyperbolically as the "ultraviolet catastrophe," Planck suggested that energy radiating from the hot body could come out only in discrete amounts—packages or quanta.

It worked. Planck had no idea that this idea would change the world for future generations, and he in fact was never comfortable with all of its implications. Nevertheless, the fruits of Planck's suggestion underlie modern life in more ways than he could have imagined. While it would take nearly half a century for computers to appear, it was the quantum application of transistors, whose existence depends intimately upon quantum physics, that made them inexpensive and ubiquitous.

It also made them small. If, like the first electronic computers, that laptop under your arm were



NIST; JILA; CU-Boulder

Figure 1. *In 1995 researchers from the Joint Institute for Laboratory Astrophysics in Colorado reported they were able to create a new state of matter—called Bose–Einstein condensate—that had been predicted by Albert Einstein after he reviewed the work of Indian physicist Satyendra Nath Bose. The researchers were able to cool rubidium atoms to less than 170 billionths of a degree above absolute zero, causing the individual atoms to condense into the same state and behave as a single entity. The graphic shows atoms condensing from less dense red, yellow, and green areas into very dense blue-to-white areas.*

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Simulating Unfamiliar States of Matter

Just as Planck could not have known the implications of his ideas, modern scientists cannot say what lines of research will change the way our own grandchildren and great grandchildren will view the world and live within it. The only safe bet is that we would be surprised. If history is a good guide, breakthroughs in the next century will most likely come from the study of ever more complex systems rather than photons or other isolated bits of matter. If so, they may stem from computer simulations such as those being performed by Dr. Tommaso Roscilde of France's École Normale Supérieure de Lyon and recently of Germany's Max Planck Institute. A team of computational scientists led by Dr. Roscilde is using the Oak Ridge National Laboratory (ORNL) Cray XT4 supercomputer, known as Jaguar, to explore the quantum mechanical phenomena that give us superconductors and superfluids.

"I think that the ultimate thing we are trying to demonstrate is not so much this or that particular behavior in the particular compound we are looking at," Dr. Roscilde noted, "but the fact that we can control a piece of condensed matter to the point that we can change the collective quantum properties of a zillion strongly interacting atoms at very low temperatures."

Dr. Roscilde and his teammates—Dr. Stephan Haas of the University of Southern California and Dr. Rong Yu of ORNL—are working on Jaguar through the Department of Energy's INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program. A grant for 1.2 million processor hours in 2008 is allowing the team to simulate a lattice of atoms to examine two extraordinary quantum phases, or states of matter.

In the first, called Bose–Einstein condensation, atoms throughout the material occupy the same state, with the same momentum, the same range of probable locations, and the same spin (figure 1). Like many properties, spin in quantum mechanics is difficult to define in classical terms, but quantum

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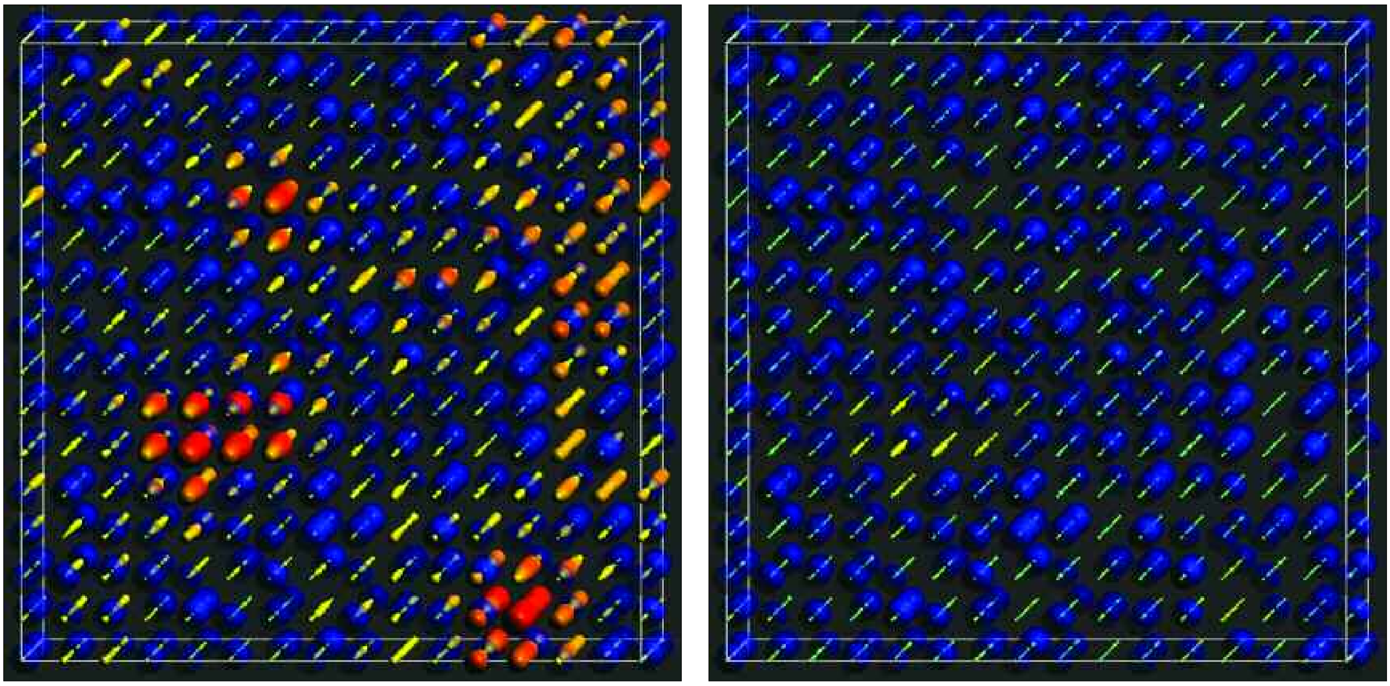

ORNL

Figure 2. *These two images illustrate the phase transition from a Bose glass to a superfluid in a diluted quantum magnet that has been exposed to an increasingly powerful external magnetic field. The size of each ball represents the local magnetization of that lattice site, which corresponds to the local density of bosonic quasiparticles. In the first image (left), the system is in the Bose glass phase at a field H = 2.79 tesla, where the quasiparticles are rare and localized in the yellow areas. At the higher field H = 2.90 tesla (right), these quasiparticles can move all over the lattice through a connected network shown in the yellow-to-red areas, giving the system a superfluid nature.*

particles can be thought of as spinning like a top. In a quantum system, this is the closest they can get to being in the same place at the same time, a state of affairs that is impossible for most matter. In the second phase being examined by the team—known as Bose glass—impurities in the material force the condensation into separate islands throughout the lattice, with atoms sharing the same state only with other nearby atoms (figure 2).

Through the Lens of Quantum Mechanics

Like Planck and many others in the last century, Dr. Roscilde and his colleagues are working in quantum mechanics, an odd, unfamiliar field focusing on the microscopic world. Quantum mechanics only rarely makes itself evident in the macroscopic world of everyday life. For the most part, our existences are governed by the 300 year old classical mechanics of Isaac Newton.

Newtonian physics does a great job of explaining the universe that we see, from the orbit of planets to the spin of a top, the arc of a football, or the flow of a river, but it begins to fall short when we take a microscopic view. In the realm of molecules and smaller, we typically must look through the lens of quantum mechanics, and that lens presents a world that seems eccentric, to say the least. The world of quantum mechanics is far less certain than its classical cousin and far more difficult to envision, often contradicting the world as we seem to experience it. Even Niels Bohr, one of the fathers of quantum mechanics, is famously quoted as saying, "Anyone who is not shocked by quantum theory has not understood it."

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Under quantum mechanics, particles sometimes behave like waves, and waves sometimes behave like particles. While it is possible in classical mechanics to characterize the state of a particle completely—using properties such as mass, charge, velocity, and position—in quantum mechanics such certainty is often impossible. Particles can be in two or more contradictory states at the same time, and we cannot know both where an object is and where that object is going.

The extraordinary states being studied by Dr. Roscilde's team (figure 3) illustrate a fundamental difference at the quantum mechanical level between two very different types of matter. According to physicists, all elementary particles fall into one of two categories, depending on their spin. Most of the matter we encounter is made up of fermions, named after the Italian physicist Enrico Fermi. Fermions include the protons, neutrons, and electrons that make up an atom, and they can be identified because they have half-integer spins (1/2, 3/2, …).

Fermions obey the Pauli Exclusion Principle, which prohibits two particles of matter from being in the same state at the same time. The other type of particles, bosons, does not. Named after the Indian physicist Satyendra Nath Bose, bosons include

Figure 3. *Researchers Dr. Tommaso Roscilde (left), Dr. Stephan Haas (center), and Dr. Rong Yu (right) are simulating Bose–Einstein condensation and Bose glass on ORNL's Jaguar supercomputer.*

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particles—such as photons—that have whole-integer spins (0, 1, 2, . . .) and unlike fermions, they gather in the same state whenever possible. This condition is known as Bose–Einstein condensation because it was first predicted by Albert Einstein after he reviewed the work of Bose.

An atom or other composite particle (that is, a particle constructed from more elementary particles such as electrons) can also behave as a boson if the combined spin of its constituents comes out to a whole integer. The best known of these composite bosons is helium-4, which becomes a superfluid when it is cooled to just over 2 degrees kelvin (that is, 2 degrees above absolute zero). A superfluid is a type of Bose–Einstein condensation, and the phase transition from regular fluid to superfluid is roughly analogous to the freezing of a liquid into a solid in classical mechanics. As a Bose–Einstein condensate, helium-4 has some very strange properties. Most notably, it has no viscosity (a measure of resistance to flow), meaning it can, for example, climb out of a test tube.

An even more bizarre composite boson—called a quasiparticle—can be produced in a quantum magnet. This is the approach being taken by Dr. Roscilde and his colleagues.

Quantum Magnets

A magnetic system might be likened to a highly ordered grove of trees, except that instead of trees there is a lattice of atomic compass magnets, all of which are able to point in the same direction (as happens in a ferromagnet). Each compass arrow reflects the spin of a single atom, which is determined by the total spin of the electrons contained in that atom. But while a classical compass arrow can point in any direction, a quantum magnet has a limited set of spin choices based on the magnitude of the quantum compass.

For the material the team is investigating (called nickel-tetrakis-thiourea), the constituent nickel atoms have a spin $S=1$; as a result, they can have a projection of -1, 0, or 1 along a given axis. For a quantum ferromagnet, the spins would all be 1, with the grove perfectly ordered. In nickel-tetrakis-thiourea, however, the spins tend rather to have a projection of 0 along a given axis, meaning they are confined to the plane transverse to the axis; and since they are in a highly quantum state in that plane, they must be thought of as pointing in all directions in that plane simultaneously. In other words, each tree is falling in every direction at the same time.

Researchers have been able to produce a condensate of quasiparticles by applying a magnetic field to a quantum magnetic material (that is, to the grove of atomic compasses). Quasiparticles are not real particles, but are rather aspects of a system that behave as though they were particles. They are not uncommon in classical mechanics. A bubble in a carbonated liquid, for instance, is a quasiparticle; it behaves as though it were a separate particle but is really just carbon dioxide displacing the liquid. In Bose–Einstein condensation, however, these magnetic quasiparticles share all the strange attributes of a boson.

For a quantum mechanical system, the state of a particle—or in Dr. Roscilde's research, the state of a quasiparticle—is conveyed by its wave function, which describes all that can be measured of it: its spin, its momentum, and the probability that it will be in a given place at a given time. All the particles in a Bose–Einstein condensate occupy the same state. This does not mean they are all in the same place simultaneously; rather it means they are all described by the same wave function. Because the function is not specific about where the particle is—instead laying out a range of possible locations—the particles will be spread out across these locations.

Dr. Roscilde's project builds from earlier work on quantum magnets at the coldest possible temperature and on the condensation of magnetic quasiparticles in them. The behaviors being simulated by the team reflect at least two aspects of a quantum system that are alien to everyday experience. In the first, the quasiparticles must be thought of as behaving

Experiments Demonstrate Quantum States

Dr. Tommaso Roscilde and his collaborators are committed to controlling the transition between Bose– Einstein condensation and Bose glass in a real-world setting. To this end Dr. Roscilde's team is collaborating with Dr. Vivien Zapf and Dr. Marcelo Jaime at the NHMFL at LANL.

The job requires very strong magnets and very cold temperatures. The NHMFL facility at LANL hosts a variety of intensely powerful magnets, and Dr. Zapf and Dr. Jaime are using a 20 tesla superconducting version for their work with Dr. Roscilde's group (figure 4). This magnet is much like the magnetic resonance imaging machine your local hospital uses to look inside your body, only ten times as powerful. The magnet itself goes in a bath of liquid helium cooled to 4K, while the sample goes into a cryogenic device known as a dilution refrigerator, which cools it further to 20 mK. This is one-fiftieth of a degree above absolute zero, or roughly −460°F.

Focusing this intensely powerful magnet on a sample of nickel-tetrakis-thiourea cooled to near absolute zero, Dr. Zapf and Dr. Jaime are able to make the spin states of each particle in the sample align, thereby producing a Bose–Einstein condensation. They will also be able to introduce impurities in the material, controlling them so that they interfere with the systemwide condensation and lead to smaller areas of localized condensation—that is, a Bose glass.

"If you have a metal, you can have something called a metal-to-insulating transition, where you're going from a conducting system to a non-conducting system," Dr. Zapf explained, "That is with electrons, which are fermions. What we're doing is looking at the analogous system for bosons."

To determine the results of each experiment, the collaborators carefully measure magnetization of the sample as well as its specific heat. Supercomputer simulations from Dr. Roscilde's team help them to interpret their results; they also guide the experimentalists as they alter the samples for eventual transition between a Bose–Einstein condensation and a Bose glass.

"That's where Tommaso comes in," Dr. Zapf explained. "They do theoretical modeling of what we expect the physical properties to look like."

both like particles and like waves. In the second, the atomic spins that are the source of the system's magnetic properties must at times be thought of as occupying more than one state at the same time.

Superposition and Schrodinger's Cat

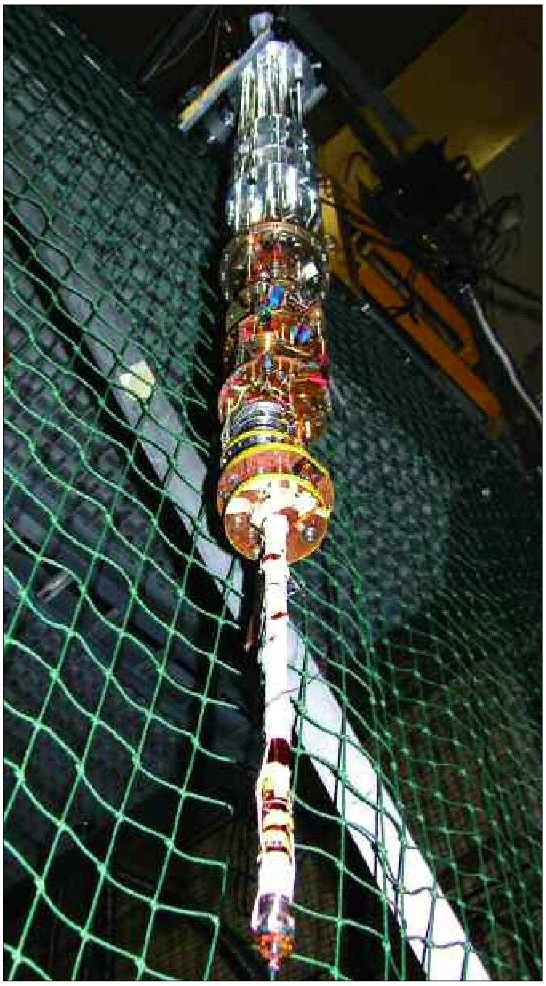
In quantum mechanics, this ability of a quantum mechanical system such as an atom to exhibit the potential for two (or more) mutually exclusive properties at the same time is known as superposition. Superposition is most famously illustrated by a thought experiment known as Schrödinger's cat, proposed in 1935 by the Austrian physicist Erwin Schrödinger. His experiment imagines a cat locked for 1 hour in a steel chamber—the inside of which cannot be observed—with a Geiger counter, a chunk of radioactive material, a hammer, and a container of hydrocyanic acid. There is a 50/50 chance one atom in the radioactive substance will decay. If it does, the Geiger counter causes the hammer to drop, breaking the container of hydrocyanic acid and killing the cat. If not, the cat lives.

According to Schrödinger, as translated by John D. Trimmer for *Proceedings of the American Philosophical Society*, "If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The psi-function (wave function) of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts."

While this example of superposition may seem ridiculous at the scale of a cat in a box, it is key to the Bose–Einstein condensate being studied by Dr. Roscilde and his colleagues. As atoms in the lattice are subjected to an increasingly powerful magnet, they change from a spin state of 0, in which their spins have zero projection along the field, to a spin state of 1, in which their spins line up with the magnetic field. As they do so, however, they go through a superposition of spin states, with a decreasing portion of the spin in the 0 state and an increasing portion in the 1 state as the magnetic field increases.

Dr. Roscilde refers to the portion that is still spin 0 as alpha, with the portion that aligns with the field (that is, the portion that is in spin 1) as beta. Going back to the grove, each tree is then both standing and fallen, with the alpha portion being in the fallen position and the beta portion being in the standing position. It is this beta portion that forms the quasiparticles, with the beta portion of each atom's spin being a portion of a quasiparticle and the total number of quasiparticles rising as the magnetic field increases. The striking aspect of the state induced by the field is that all the particles have the same alpha and beta coefficient—that is, the standing portion of each tree is exactly the same. Therefore, a single wave function can potentially describe a large number of quasiparticles, meaning they are in a condensate.

Researchers have found that it is far more difficult to form such a condensate in a material that is not



LANL

Figure 4. *This dilution refrigerator at Los Alamos National Laboratory is able to cool a sample to 20 mK (1/50 of a degree above absolute zero, or roughly −460°F). The blue object in the background is a 20 tesla superconducting magnet, roughly 10 times more powerful than the magnet on a typical magnetic resonance imaging machine.*

Dr. Roscilde's team is using computer simulation to introduce disorder in a quantum magnet, thereby creating Bose glass through a process known as doping.

pure, either because there are vacancies in the lattice of the material or because some sites in the lattice are occupied by molecules from different materials—impurities. In our grove, a tree missing from the carefully laid out rows of trees would be a vacancy, while a tree of a different type (oak instead of pine, for instance) would be an impurity.

These impurities are far more important in a quantum mechanical system than they would be in a classical system. A similar modification of a classical system might not be much of a hindrance to motion, since classical particles would be able to flow around the impurities. In a quantum system, however, each particle also behaves as a wave. Just as a rock poking out of a pond scatters a wave in the water, an impurity in the magnetic material will scatter the waves of the quasiparticles, partly transmitting them and partly reflecting them. These transmitted and reflected waves interfere with one another, with the result that separate condensates gather in areas of the lattice that are relatively free of impurities. While particles will be in the same state as nearby particles, they will not be in the same state as the other islands of condensate. This is known as a Bose glass.

Dr. Roscilde's team is using computer simulation to introduce disorder in a quantum magnet, thereby creating Bose glass through a process known as doping. The team starts out with a perfect magnet and adds impurities, creating a Bose glass where there had been a Bose–Einstein condensate. What the team is finding is that the system will eventually overcome the impurities introduced into it as the magnetic field reaches a critical level. At this point, the number of quasiparticles has increased to the point at which they push each other out of their localized state and a systemwide Bose–Einstein condensate is restored.

The work is at the cutting edge of condensed-matter science.

"I find that in this particular instance of a study of a solid-state system, you're really trying to tailor matter to a level of control that was unthinkable a few decades ago or even a few years ago," Dr. Roscilde said. "What you have is a system where, in principle, by controlling the disorder—which you can to a fair amount of accuracy—you can tune the system among completely exotic phases that have no analog in classical systems."

From Computation to Experiment

While Bose–Einstein condensates have been observed experimentally, Bose glass has not.

The team uses a quantum Monte Carlo technique with ORNL's Jaguar system to predict the proper doping of the material for a Bose glass as well as the ideal temperatures and magnetic field for producing the phase.

Taking the Quantum Monte Carlo Approach

The universe is a very complex place. This fact of life imposes some daunting challenges for computational scientists, many of whom must simulate systems that are very difficult to understand and model. By repeatedly sampling these difficult systems, though, Monte Carlo algorithms give researchers an opportunity to solve intensely complex problems with a minimum of uncertainty.

The Monte Carlo method was first developed by scientists working on the U.S. Manhattan Project and has been applied to a wide range of problems, from molecular biology to financial modeling. In general, it does its job in three steps. First, the program generates a random sequence of numbers—or rather, a pseudorandom sequence, since no computer algorithm can generate truly random sequences. Second, it uses this random sequence to generate a multitude of system samples. Finally, it tallies the outcomes of these samples to come up with a result.

Monte Carlo algorithms are well suited to computational problems that involve interdependent systems, where a change to one element can have repercussions too complex to anticipate. This is the case for strongly correlated quantum spin systems subject to a magnet field, such as the systems being simulated by Dr. Tommaso Roscilde of France's École Normale Supérieure de Lyon and his teammates, Dr. Stephan Haas of the University of Southern California and Dr. Rong Yu of ORNL. The team is using the ORNL Cray XT4 Jaguar supercomputer (figure 5) to probe two extraordinary quantum phases, known as Bose–Einstein condensate and Bose glass.

The team uses a quantum Monte Carlo approach known as stochastic series expansion, in which the algorithm is able to assign importance to the samples in order to provide the most useful information and the quickest result. This approach has been shown to be very robust in simulations similar to those being produced by Dr. Roscilde's team, in which large quantum bosonic spin systems are being simulated with varying external magnetic field strengths.

The simulations being performed by Dr. Roscilde and his team look at novel quantum phases in disordered quantum spin systems to which magnetic fields have been applied. In particular, they look at the nature of the transition from Bose–Einstein condensate to superfluid as the magnetic field strength increases and as temperature varies above and below a critical point.

A typical simulation will have around 1,000 bosonic quasiparticles, with inputs such as temperature, magnetic field, and concentration disorder. For each system size, the simulation typically looks at 20 or so applied magnetic field values. The temperature is systematically lowered until the physical properties do not depend on temperature. Five or so system sizes are surveyed to determine the dependence on system size, and a grid of temperature points is examined to determine the likely temperature range for these extraordinary quantum states in which the researchers are interested. Given the number of systems and system values that must be calculated, such a simulation would be impossible without a massively parallel supercomputer such as the ORNL Cray XT4, Jaguar.

Dr. Roscilde and his teammates are collaborating with Dr. Vivien Zapf and Dr. Marcelo Jaime at the National High Magnetic Field Laboratory (NHMFL) at Los Alamos National Laboratory (LANL) to change that (sidebar "Experiments Demonstrate Quantum States," p54). The LANL facility is one of three campuses of the NHMFL and provides the intense magnetic field needed to demonstrate these quantum phases.

Dr. Roscilde believes his colleagues at LANL will be able to demonstrate a Bose glass experimentally in the same manner that his team is inducing it computationally. The two teams are using the material nickel-tetrakis-thiourea because it has an unusual combination of properties; namely, it exhibits Bose–Einstein condensation and can be doped in a controlled manner.

Dr. Roscilde's team is able to guide these experiments by investigating theoretical models for the material and predicting the circumstances under which the Bose glass phase should be seen. The team uses a Quantum Monte Carlo technique with ORNL's Jaguar system to predict the proper doping of the material for a Bose glass as well as the ideal temperatures and magnetic field for producing the phase (sidebar "Taking the Quantum Monte Carlo Approach").

The computational scientists are also able to predict the identifying features, or signatures, that will demonstrate that the experiment was able to achieve a Bose glass. The computer simulation calculates all aspects of the system that can be measured in an experiment, such as magnetization along the applied field and the specific heat of the system.

Dr. Roscilde says the collaboration demonstrates how computation and experiment can use their individual strengths to buttress one another. On the one hand, Dr. Roscilde and his team have the advantage of being able to look into the system at both the macroscopic level of measurable properties and a microscopic level that cannot be viewed through experiment. On the other hand, these phases are

NCCS AT ORNL

Figure 5. *Jaguar, the Cray XT4 supercomputer at ORNL.*

only imperfectly understood, and the computational scientists must work very closely with experimentalists. After all, a model that does not reflect the system it is modeling is worthless.

"If the theoretical and the experimental data match up for the macroscopic properties, one gains from the theoretical study the fundamental information on the microscopic physics at the basis of the observed behavior," he noted.

"Of course, the interaction with experimentalists is not just one way; the physics of the real materials might show unexpected features that have to be incorporated in the calculations at a later stage. Our knowledge of the models describing the behavior of real materials is always necessarily incomplete, and when we expose a material to a significant perturbation such as doping, some of the parameters we think we know might need to be reconsidered."

Dr. Roscilde and his team also hope to answer some open questions that remain regarding the physics of Bose glass. The most important of these may focus on how a material moves from a Bose glass phase to a Bose–Einstein condensate with an increasingly intense magnetic field.

"The full picture of this transition is still unknown," he noted, "and it is fundamentally encoded in a set of numbers (so-called critical exponents) which govern the dramatic way in which some macroscopic quantities change at the transition. The knowledge of these exponents is fundamental to shedding light on quantum phase transitions taking place in presence of disorder, which is one of the most challenging issues in condensed-matter physics."

Towards Practical Applications

As with much fundamental research, such as Planck's work more than a century ago, it is impossible to say whether work on Bose–Einstein condensation and Bose glass will bring with it any practical benefit beyond a deeper understanding of the universe in which we live. At this point, we've not even seen a Bose glass outside of computer simulation.

Nevertheless, studies of what may seem like the odd boundaries of physics have already led to world-changing advances. Witness Dr. Albert Fert of the Université Paris-Sud in France and Dr. Peter Grunberg of the Jülich Research Center in Germany, this year's winners of the Nobel Prize in physics. In 1988 the two independently discovered a quantum effect known as giant magnetoresistance. In subsequent years, this discovery has been credited with revolutionizing data storage and, among other things, making modern MP3 players possible.

Dr. Roscilde is quick to point out that there are, so far at least, no obvious applications looming on the horizon for the work he and his peers are doing into Bose–Einstein condensation and Bose glass. For one thing, he notes, practical applications of quantum mechanics so far have typically relied on insights into the behaviors of single particles. His work, on the other hand, seeks insights into the behavior of systems of particles.

"There are some fields that are more mature for application and some that need more work," he explained. "So far, applications that are based on quantum effects are typically based on the knowledge of a single quantum particle. It doesn't so much rely on the knowledge or behavior of a collective quantum state of many particles."

Dr. Roscilde noted also that a device based on quantum systems would likely be very different from existing technologies.

"You have to think hard what to make out of these systems," he noted. "It's not just that once you know them, you know what to make out of them.

"You cannot just think of a new device in terms of traditional devices. You cannot think, 'Okay, let's make a transistor out of this.' You have to totally think of new functionalities. If you keep going with the same paradigm in mind, you probably don't need all this control over a complex collective state of many particles. You need a device that's fundamentally based on the behavior of many particles at the same time." ●

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