

A quintessential quantum simulator takes a 10 000-fold leap

Experiments on the fermionic Hubbard model can now be made much larger, more uniform, and more quantitative.

A universal quantum computer—capable of crunching the numbers on any complex problem posed to it—is still a work in progress. But a type of specialized analog quantum computation may be on the cusp of achieving some groundbreaking results, thanks to new work by researchers in Jian-Wei Pan's group at the University of Science and Technology of China (USTC).¹

Pan, Yu-Ao Chen, Xing-Can Yao, and other group members sought to study the behavior of the fermionic Hubbard model (FHM), a stripped-down theoretical representation of electrons in a solid. Stripped down though it may be, it captures much of the subtle physics of strongly correlated many-body systems, and it's thought to be relevant to perhaps the grandest many-body challenge of all: the enduringly mysterious mechanism of high-temperature superconductivity in cuprate ceramics and related materials. Unfortunately, the model, when treated as a math problem, defies even numerical solution for all but the simplest cases.

The USTC researchers treated the model as a physics problem: Using optical traps, they built a lattice of ultracold atoms designed to obey the FHM Hamiltonian, and they watched how it behaved as they tuned the system's parameters. They're not the inventors of that approach; several groups have been working on it for years (see *PHYSICS TODAY*, October 2010, page 18). In 2017 Harvard University's Markus Greiner and colleagues made a splash when they observed antiferromagnetic correlations—a checkerboard pattern of up and down spins—that spanned their 2D lattice of 80 optical traps.² (See *PHYSICS TODAY*, August 2017, page 17.) It was one of the first clear signs

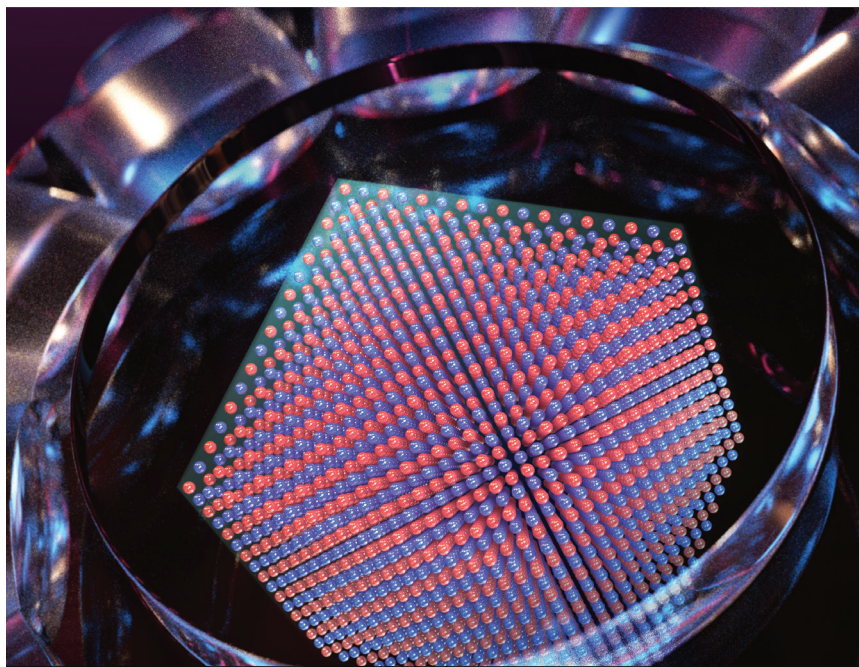


FIGURE 1. ANTIFERROMAGNETICALLY ORDERED PARTICLES are represented by red and blue spheres in this artist's impression. The array shown here is a cube with 17 particles on each side, but a new experiment probed a cold-atom lattice more than five times as large in each dimension.¹ A major experimental challenge was keeping the conditions uniform over such a large system. (Courtesy of Chen Lei.)

that FHM experiments might be nearing a regime in which researchers could observe new physics. But the benchmark has been unsurpassed for seven years.

The new experiment now shows 3D antiferromagnetic ordering, as illustrated in figure 1, across a lattice of some 800 000 optical traps. The system is big enough—and uniform enough—for the researchers to make quantitative measurements, including studying the system's critical exponents, key indicators of the underlying physics. “This paper came out of the blue,” says Randy Hulet of Rice University. “It’s really rejuvenated the optical-lattice field.”

Stalemate?

The many-electron wavefunction of a solid is extremely complicated. Electrons move continuously in 3D space, influenced by the potential-energy landscape

of the atomic nuclei (which themselves are also moving) and the long-range Coulomb repulsion of all the other electrons.

In contrast, the FHM is admirably simple. Its fermionic particles occupy only the discrete nodes of a lattice, and they interact only with particles on the same node. (Typically, the fermions are taken to have spin $\frac{1}{2}$, and each node can accommodate at most two particles: one with spin up and one with spin down.) The particles can hop to neighboring nodes, but they can't change their spin states. The system is characterized by only a handful of tunable parameters: the interaction energy of particles on the same node, the energy required to hop nodes, the temperature, and the average density of particles per node.

Given that simplicity, it's perhaps surprising that the FHM captures so many

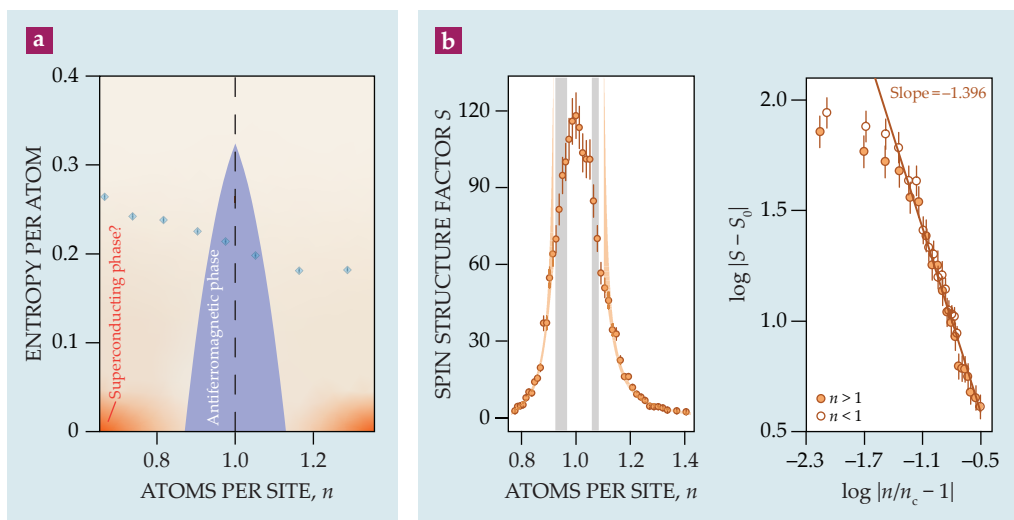


FIGURE 2. EXPLORING THE PHASE DIAGRAM of the 3D fermionic Hubbard model. **(a)** The blue dots show the entropy per atom that researchers could achieve as a function of the atom density n . The experiment could probe the phase transition into and out of the antiferromagnetic phase, but reaching the putative superconducting phase will require cooling the system much further. **(b)** Near $n = 1$, the spin structure factor S is large. Outside of the antiferromagnetic phase, whose boundaries n_c are estimated to be somewhere in the gray bands, S decays with a power-law dependence. As shown in the log-log plot on the right, the power-law scaling is consistent with the expected critical exponent, 1.396. (Adapted from ref. 1.)

of the real effects of solid-state physics, such as antiferromagnetism. When the same-node interaction is repulsive, the temperature is low enough, and the particle density is near the so-called half-filled level of one particle on average per node, particles settle into a state in which exactly one sits at each node. Even though they're not sharing nodes and therefore not interacting with one another, the subtleties of quantum mechanics and Fermi-Dirac statistics drive them toward a pattern of alternating spins.

The antiferromagnetic phase is also observed in the cuprates and other superconductors near zero doping—that is, when the material composition provides neither extra electrons nor holes to carry charge through the otherwise superconducting layers. The FHM's antiferromagnetism is a tantalizing hint that a superconducting phase may be lurking nearby. But to get there, researchers need to move to still lower temperatures and away from half filling, and that's where the understanding breaks down.

The half-filled FHM is one of the few cases that theoretical studies can grapple with reasonably well. Away from half filling, theorists run up against the sign problem: The integrals involved are dominated by large positive and negative contributions that almost, but don't

quite, cancel out, so they're extremely difficult to calculate accurately. Meanwhile, experimenters have been stalled in their quest for lower temperatures.

Double attack

Fermionic atoms in optical traps are a reasonable approximation of the FHM's particles on discrete lattice nodes. And arrays of equally spaced optical traps easily emerge—in 1D, 2D, or 3D lattices—from the interference patterns of pairs of counterpropagating laser beams.

But that setup requires exceptionally low temperatures. To mimic the physics that arises in real materials at tens to hundreds of kelvin, a trapped-atom FHM experiment must be cooled to tens of nanokelvin—near the limit of what cold-atom physicists can currently achieve.

Another big limitation is the system uniformity. Laser beams as typically generated have Gaussian profiles: They're brightest in the center and fade away around the edges. As a result, in a 2D or 3D lattice of traps made from Gaussian beams, the traps in the middle are deeper than those around the periphery. In an experiment on more than a few dozen of those traps, it's likely that different parts of the system would be in completely different phases.

The USTC researchers took on both those challenges. For the latter, they built custom-designed diffractive optical elements to convert their Gaussian beams into flat-top beams with uniform intensity over almost the entire beam profile. With three pairs of flat-top beams, they formed a uniform lattice nearly 100 sites wide in each dimension, for 800 000 sites total.

But the benefits of homogeneity don't stop there. In a typical FHM experiment, researchers hold the atomic gas in a single large Gaussian trap before loading it into the lattice of smaller traps. The trap is deepest in the center, so the gas is densest there—and the inhomogeneity of the gas density is a source of entropy in the lattice.

What Pan, Chen, Yao, and colleagues did instead was hold the gas in a box trap: a hollow cylinder made of light, whose walls

repel the atoms and keep them inside. By allowing the gas to equilibrate to a uniform density over the volume of the trap, they could load it into the lattice much more uniformly. "In retrospect, that's obvious, but they were the first to realize it," says Hulet. The more uniform loading leads to significantly lower entropy—by at least a factor of two—and therefore lower temperature.

King's gambit

With a 3D lattice that's large, cold, and uniform, the researchers were uniquely positioned to observe something that had never been seen before in the FHM: the phase transition to antiferromagnetic order. Importantly, although Greiner and colleagues had seen antiferromagnetic correlations in their 2D experiment, they didn't see an actual antiferromagnetic phase, which doesn't even exist in 2D. Rather, the antiferromagnetic correlations start small and gradually spread across the 2D system at lower temperatures. When Greiner and colleagues saw a checkerboard pattern spanning their 80-site lattice, it was because the model's correlation length had grown larger than the system they were looking at.

On the other hand, whereas Greiner and colleagues used a quantum gas

microscope to see the checkerboard pattern directly, that option wasn't available to the USTC researchers. Instead, they used Bragg scattering to measure the spin ordering in their 3D lattice, similar to how x-ray scattering probes the ordering of atoms in a real crystal.

Figure 2 shows one of their experiments that studied the antiferromagnetic phase transition. Panel a is a sketch of the system's phase diagram in terms of entropy (related to temperature) and the particle density n ; the antiferromagnetic phase forms a symmetric dome on either side of the half-filled state $n = 1$. The series of blue dots shows how the researchers tuned n to probe a slice of phase space that cuts through the antiferromagnetic dome.

Panel b shows the USTC researchers' measurements of the spin structure factor S , which quantifies how well-ordered the spins are. Near $n = 1$, S is large, as expected of an antiferromagnetic phase. But outside of the phase boundaries, which the researchers estimate to lie somewhere in the gray bands, S doesn't abruptly drop to zero. Rather, it tails off with a power-law dependence.

The power law is defined by a critical exponent, and there are only a few values the exponent could plausibly take. A wide variety of seemingly disparate physical systems fall into a small number of universality classes, each with its own characteristic scaling behavior (see *PHYSICS TODAY*, July 2023, page 14). The FHM is thought to belong to the same universality class as the 3D Heisenberg model, which would give it a critical exponent of 1.396. But that's never been confirmed, because the FHM phase transition had never been observed before.

When the researchers drew a line with slope -1.396 , they found that it agreed reasonably well with their data in the log-log plot in figure 2b. Importantly, though, the experiment doesn't constitute a measurement of the critical exponent. "Accurately determining the critical exponent of a power-law function requires making measurements over several orders of magnitude," explains Yao. "In our current work, we did not fulfill that condition. But in the future, we hope to determine the value precisely."

Your move

Pan, Chen, Yao, and colleagues have performed the most quantitative and informative FHM experiment to date, but there's much more to be done. The superconducting phase, if it exists, lies at temperatures even lower than the researchers have achieved, and they'll need further experimental improvements to access it.

If and when researchers do reach the superconducting phase, the next step will be to perform detailed experiments to try to uncover the mechanism by which the fermionic particles combine into bosonic pairs that condense into a superfluid. Part of the reason that cuprate superconductivity has been so enigmatic is that there's no way to tune individual properties in isolation. Just to change the charge-carrier density, for example, it's necessary to make a new sample with a different chemical composition, which changes other properties in tandem.

In the FHM, on the other hand, changing the particle density is as straightforward as reloading the lattice with more

or fewer atoms. Other parameters can be tuned too, including those that take the model beyond the classic FHM to simulate effects such as phonons or spin fluctuations. By testing how each parameter does or doesn't contribute to superconductivity, researchers could finally uncover the mysterious electron-pairing mechanism.

But understanding superconductivity isn't the only goal. Strongly correlated electron systems give rise to many other physical phenomena, some of which show up in the FHM at the temperatures researchers can achieve already. "Due to the difficulty in numerical calculations, little is currently known about the 3D FHM at low temperatures and away from half filling," says Yao. "Mapping out its phase diagram is important in its own right."

And the USTC group won't be the only one working on the FHM. Box traps, the key to lowering the quantum gas's entropy and temperature, are an established technology, so now that their importance for creating low-entropy gases is known, other groups can start using them too. The diffractive optical elements used to create the flat-top beams were custom designed, but similar products are available commercially. "It will absolutely be possible for other groups to replicate these results," says Hulet. "Pan's group is ahead of everybody else, but only by a few months."

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References

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A titanium:sapphire laser on a chip

The miniaturized laser has a lowered output power suited for many applications without sacrificing stability and tunability.

A standard tool in optics labs, titanium-doped sapphire lasers are valued for their ability to be precisely tuned across a wide wavelength range. In Stanford University's Nanoscale and Quantum Photonics Lab, led by Jelena Vučković, researchers use ta-

bletop Ti:sapphire lasers to excite artificial atoms in solid-state quantum optics experiments.

But the lasers typically require a bulky, expensive, high-power pump laser. And the Vučković group, like many others, require only a fraction of

the Ti:sapphire's output power: The researchers in the Nanoscale and Quantum Photonics Lab often end up attenuating the laser from watts to microwatts.

Dissatisfied with the standard laser setup's wasted power, high cost, and other shortcomings, the Stanford researchers saw an opportunity to miniaturize. Vučković is no stranger to shrinking lab components: She and members of