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Visualizing the Universe in Any Material

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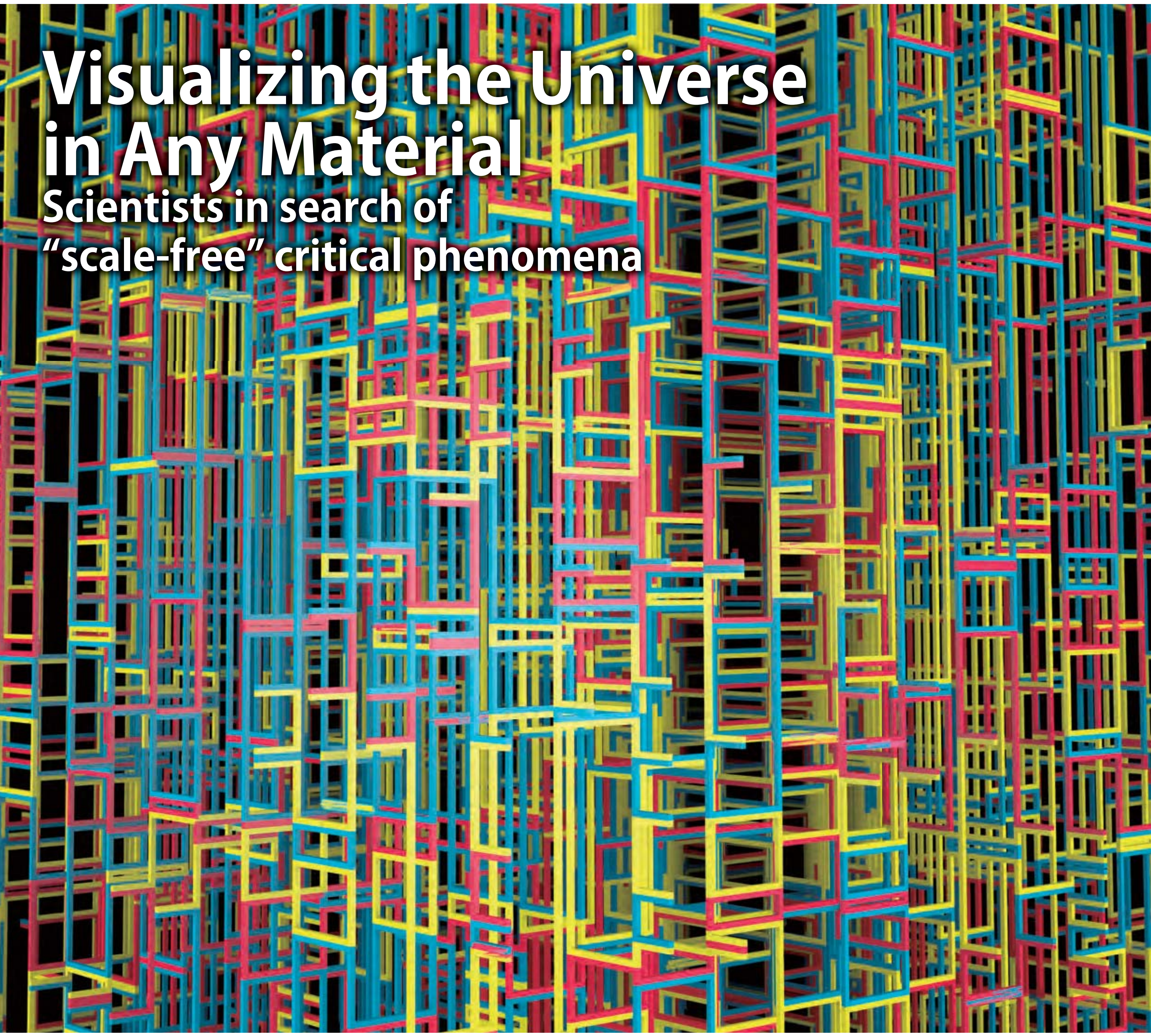

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Interview

Visualizing the Universe in Any Material

Scientists in search of “scale-free” critical phenomena

Kenji Harada

Assistant Professor of the Graduate School of Informatics, Kyoto University

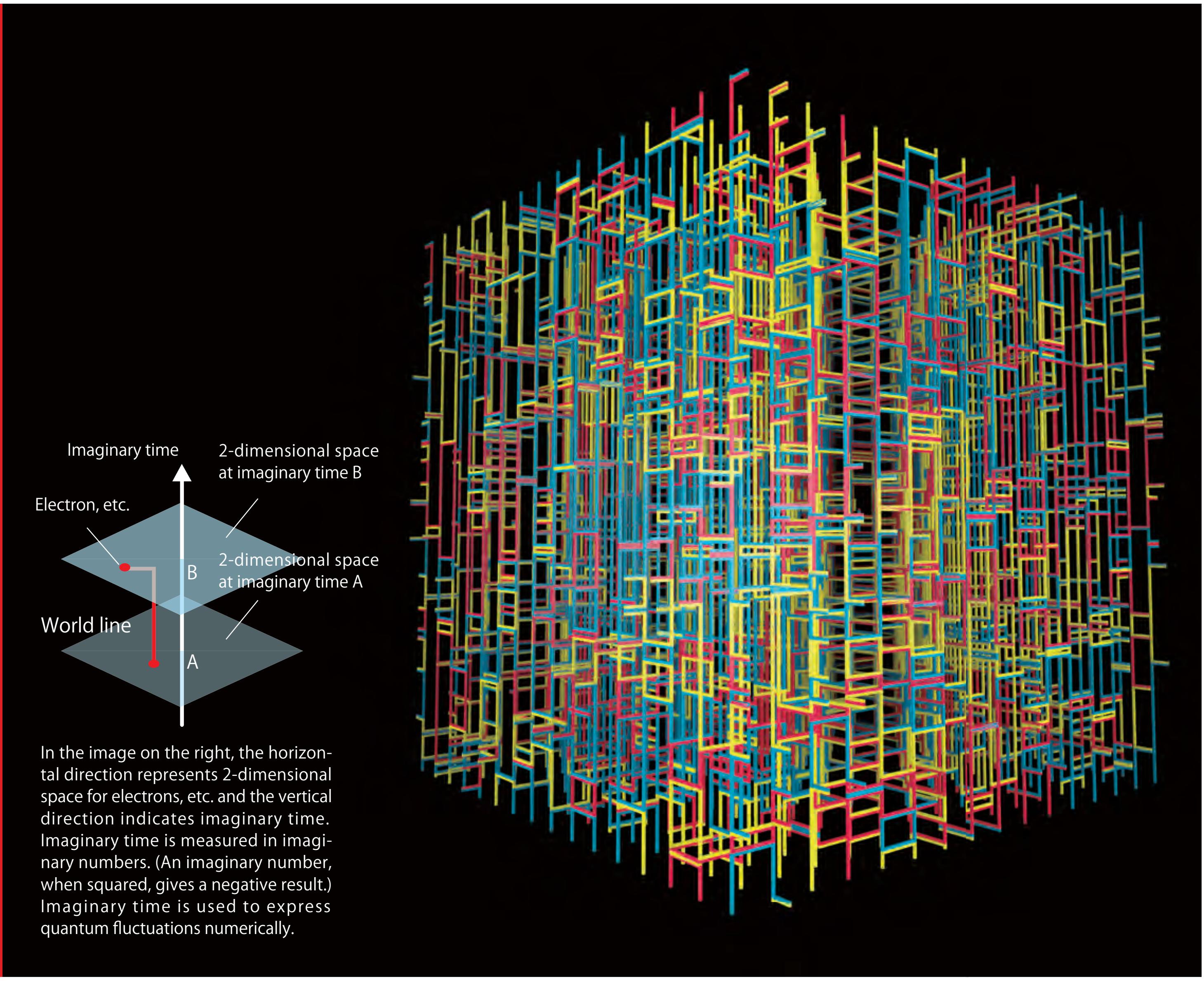


Fig. 1 Deconfined quantum critical phenomenon and the state of world line
Colored lines in the figure show the paths (world lines) of electrons and other particles in imaginary time-space. Verification of deconfined quantum critical phenomena has its basis in data from world line calculations.

Harada is a member of a team with a mission to discover new critical phenomena, for which they are making full use of K and other supercomputers. The phenomena under investigation represent a form of phase transition, where a substance in one state suddenly changes to another state under a particular set of conditions. Such phenomena are not limited by physical scale and are thought to occur in everything from elementary particle, the smallest unit of matter, to the universe itself.

Difficulties in simulating the quantum world

Looking back at his first involvement in computers, Harada says, "In high school, we built a computer graphics program as an extracurricular project. During the endeavor, I encountered ray tracing, a method of computing and tracking the light reaching our eyes from reflected objects."

"Our CG program was simple because the computer's performance was limited, but I was deeply impressed by its potential to create a seemingly real world of light beams and objects whose images could not easily be distinguished from real objects."

Today, Harada is engaged in simulating infinitesimally small elements, such as atoms and electrons, on supercomputers. "It's impossible to simulate the world of quanta on current mainstream computers," he says. "Even an electron is so unstable that it is continually fluctuating. From this fact, it appears that there occur in the quantum world various events that are hard for us to imagine happening. Our job is to find ways to simulate a range of phenomena occurring in substances that are in line with certain quantum properties."

But this task entails an enormous number of calculations. Imagine simulating a state where the number of atoms has increased 10 times more than previously. The number of calculations soars by a margin of 10 raised to the power 10, not simply by 10 times."

To overcome this difficulty, Harada's team carefully chooses sample substances and phenomena that are easy to compute, and the group constantly reviews its calculations and procedures so as to obtain the best possible results from a quantum-world simulation.

"It's a difficult but really interesting assignment," says Harada.

Two different critical phenomena occurring concurrently

One kind of phenomenon Harada is simulating is called critical phenomena, a form of phase transition.

So what is phase transition? "For example, a phase transition occurs when water changes to ice at 0℃, or when some substances turn magnetic at a certain level of pressure or temperature. Phase transition refers to a situation where one substance undergoes a sudden change in its properties," explains Harada. Is there a difference between a phase transition, like the water-to-ice change, and critical phenomena?

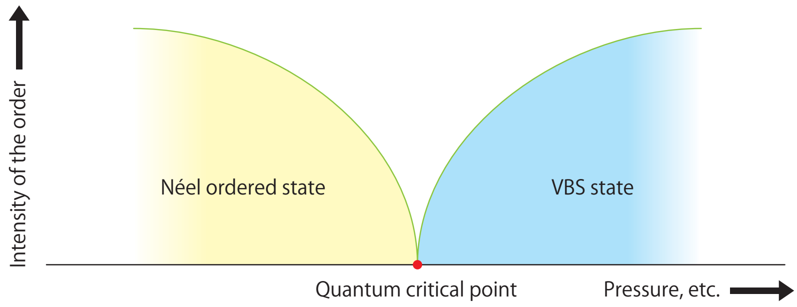
"To explain further, a phase transition takes place—water to gas, for instance—when a substance's parameters such as temperature or pressure changes at a critical point in the boundary between the two phases or states," says Harada. "At this critical point the two phases can become indistinguishable, the boundary disappears and the substance undergoes a drastic change. The theory of critical phenomena seeks to explain this drastic change. And because critical phenomena are not limited in terms of physical scale, they are scale-free. The same kind of critical phenomena occurring in materials we understand well are also believed to happening at the level of elementary particles, the smallest units of matter, as well as whatever else makes up our entire universe. Research on critical phenomena, therefore, merits much attention."

In theory, substances are subject to innumerable kinds of critical phenomena, but only a few have been reported for two- and three-dimensional substances. A critical phenomenon, then, can be thought of as a buried diamond—very hard to discover. Against this backdrop, Harada and his colleagues are investigating a phenomenon, called "deconfined quantum criticality," which takes place very rarely.

Deconfined quantum criticality involves electron spin and takes place at absolute zero (-273.15℃). Electron spin, the source of magnetic force generation, has a direction. And it is when many electrons spin in the same direction that a material turns magnetic.

With a deconfined quantum critical phenomenon, the pattern of electron-spin direction collapses suddenly under a particular circumstance, and then the columnar arrangement of entangled electron-pairs appears (see Fig. 2). This indicates two different critical phenomena are occurring at the same time, from the point of symmetry.

"To clarify," says Harada, "imagine a bucket of magnetized water. If you keep applying pressure to the water, the liquid



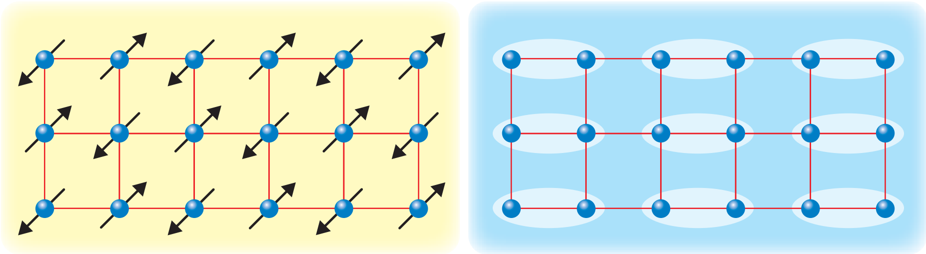


Fig. 2 Deconfined quantum critical phenomenon
Compared to the Néel ordered state where electron-spin directions alternate, these spins are paired up in the Valence Bond Solid (VBS) state. If a substance shows no change in its overall state after conducting a certain operation, then it is "symmetrical" to the operation. In fact, the Néel ordered state shows no change even following a 90-degree rotation of lattices. However, it does change when the electron-spin directions are both rotated at the same time. Therefore, the Néel ordered state spontaneously breaks the rotational symmetry of spin directions, not the 90-degree rotational symmetry of lattices. On the other hand, the VBS state breaks the symmetry of the lattices, not the spin direction of the electrons. Upon increasing the pressure applied to a sample substance, the broken rotational symmetry of electron- spin directions in the Néel ordered state is switched to the broken 90-degree rotational symmetry of lattices in the VBS state at the transition point. Given critical phenomena are interpreted as representing spontaneous symmetry breaking, it is thought that two different critical phenomena occur collectively and in mutually reverse directions at the transition point between Néel and VBS ordered phases when symmetry is broken.

Before he was fully aware of the fact, Harada had become a scientist. The transformation happened in a graduate school environment where he received much encouragement from senior colleagues in different fields, and especially after he worked with a research supervisor who impressed with his vigor and passion in building a parallel computer from scratch.

(Harada poses in front of Sekirei, a supercomputer at The University of Tokyo's Institute for Solid State Physics)

changes to ice at a certain point while losing its magnetism. Two seemingly unrelated phenomena apparently occur at the same time. A deconfined quantum critical phenomenon is similar to this, where two kinds of critical phenomenon occur in mutually reverse directions simultaneously."

There is much debate about deconfined quantum critical phenomenon, which cannot be explained by conventional theories.

K has the power to verify deconfined quantum criticality

In searching for incidents of deconfined quantum criticality, Harada's group has made simulations of certain materials and changed various parameters affecting them, such as the level of applied pressure. The researchers eventually discovered that electrons in small amounts of these materials exhibit a change in electron spin, a phenomenon similar to deconfined quantum criticality (see Fig. 1 and Fig. 3).

To verify this apparent critical phenomenon, the group has to substantiate if the same electron-spin change occurs in a larger portion of these substances. The task, however, requires a great number of calculations. So Harada has employed the K computer, one of the world's fastest supercomputers, and the Sekirei supercomputer at The University of Tokyo's Institute for Solid State Physics.

"There's a high probability, about 80 percent, that computer-detected changes will be deconfined quantum critical phenomena, while twenty percent of them may not be," says Harada. "We assume that at the very moment a change begins (the quantum critical point), previously confined virtual particles (spinons) are set free and start to move about in these substances. Spinons apparently help hook up the two different phenomena and then cause them to occur at the same time.

"We'll work to verify this unique phenomenon by simulating free-moving spinons on supercomputers," he added.

Powerful aid to research on elementary particles and the cosmos

What's the importance of critical phenomenon research? "Whenever my wife asks how my research will be useful, I'm at a loss for an answer," Harada says with a chuckle.

Given the fact that deconfined quantum criticality occurs only at absolute zero, results of the related research are unlikely to lead directly to the development of equipment and materials used for practical purposes. Nevertheless, they will certainly have a huge impact on our understanding of physics.

Notes Harada: "Deconfined quantum criticality has long been considered to take place in elementary particles. Calculations based on the latest elementary particle theories are more complex than those of sample substances we've used. Such criticality, therefore, has yet to be fully verified."

"But if it is verified for these substances, the phenomenon can be considered to be happening across all physical scales, from elementary particles to the universe itself, which will contribute greatly to advancing our understanding of particle physics and cosmology. We would be able to see aspects of the universe in the tiniest of substances. That's one of the most alluring prospects of conducting research on critical phenomena."

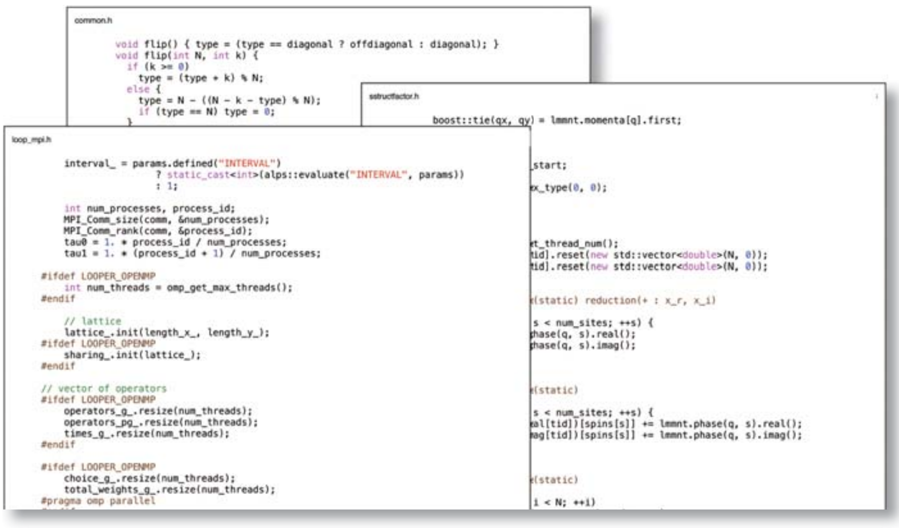


Fig. 3 Part of the computing program to verify deconfined quantum criticality (based on the ALPS/looper)

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