Quasicrystals: Somewhere between order and disorder

Professionally speaking, things in David Damanik's world don't line up – and he can prove it. In new research that's available online and slated for publication in July's issue of the *Journal of the American Mathematical Society*, Damanik and colleague Serguei Tcheremchantsev offer a key proof in the study of quasicrystals, crystal-like materials whose atoms don't line up in neat, unbroken rows like the atoms found in crystals.

Damanik's latest work focused on a popular model mathematicians use to study quasicrystals. The research, which was 10 years in the making, proves that quasicrystals in the model are not electrical conductors and sheds light on a little-understood corner of materials science.

"This is the first time this has been done, and given the broad academic interest in quasicrystals we expect the paper to generate significant interest," said Damanik, associate professor of mathematics at Rice University.

Until 1982, quasicrystals weren't just undiscovered, they were believed to be physically impossible. To understand why, it helps to understand how atoms line up in a crystal.

In literature dating to the early 19th Century, mineralogists showed that all crystals -- like diamond or quartz -- were made up of one neat row of atoms after another, each row repeating at regular intervals. Mathematicians and physical chemists later showed that the periodic, repeating structure of crystals could only come in a few fixed arrangements. This was elegantly revealed in the early 20th Century when crystals were bombarded with X-rays. The crystals diffracted light into patterns of spots that had "rotational symmetry," meaning that the patterns looked exactly the same when they were spun partway around. For example, a square has four-fold rotational symmetry because it looks exactly the same four times as it is spun a full turn.

X-ray crystallography reinforced what physicists, chemists and mathematicians already knew about crystals; they could yield patterns of spots with only two-, three-, four- or six-fold rotational symmetry. The physics of their lattices permitted nothing else.

All was well until 1982, when physicist Dan Shechtman did an X-ray diffraction study on a new alloy he'd made at what is now the National Institute of Standards and Technology. The pattern of spots looked like those made by crystals, but it had five-fold rotational symmetry, like a pentagon – something that was clearly forbidden for a periodic structure.

The alloy -- which was quickly dubbed quasicrystal -- attracted intense scientific interest. Dozens of quasicrystals have since been made. Though none of their structures have yet been solved, scientists and mathematicians like Damanik are keen to understand them.

"Mathematically speaking, quasicrystals fall into a middle ground between order and disorder," Damanik said. "Over the past decade, it's become increasingly clear that the mathematical tools that people have used for decades to predict the electronic properties of materials will not work in this middle ground."

For example, Schrödinger's equation, which debuted in 1925, describes how electrons behave in any material. But for decades, mathematicians have been able to use just one of the equation's terms -- the Schrödinger operator -- to find out whether a material will be a conductor or an insulator. In the past five years, mathematicians have proven that that method won't work for quasicrystals. The upshot of this is that it is much more complex to actually run the numbers and find out how electrons behave inside a quasicrystal. Supercomputers have been used to actually crunch the numbers, but Damanik said computer simulations are no substitute for a mathematical proof.

"Computer simulations have shown that electrons move through quasicrystals -- albeit very slowly -- in a way that's markedly different from the way they move through a conductor," Damanik said. "But computers never show you the whole picture. They only approximate a solution for a finite time. In our paper, we proved that electrons always behave this way in the quasicrystal model we studied, not just now or tomorrow but for all time."

Source: Rice University