SUPERHEROES 4 SCIENCE

QUANTUM RIPPLES IN GRAPHENE

When you spread a freshly ironed tablecloth on the table, it seems to be perfectly flat and smooth. However, in the microworld of atoms, things work differently. Thin membranes that are akin to a tablecloth can ripple by themselves, as long as they are sufficiently thin.

To understand this we turn to physics, which studies the microworld. Let us consider the thinnest material we can imagine. Since all matter consists of atoms, the lowest thickness a material can have is one atom. The first people to make such a material were physicists A. Geim and K. Novoselov, who used duct tape to tear away a one atom thick layer from graphite – pencil lead. They called the layer graphene, and so created the first sample of a two-dimensional material. It is two dimensional, because its thickness is much smaller than its width and length. For their discovery, which started a new era in physics and technology, they were awarded the Nobel Prize in physics in 2010. Graphene is considered very promising in electronics, due to its unusual electrical properties.

Graphene also has other extraordinary properties, such as its high mechanical strength and heat conductivity. Today graphene is no longer the only two-dimensional material, there are many others, and the list of them keeps expanding. Furthermore, different two dimensional materials can be stacked on top of each other to create new materials with interesting properties and potential for use in all kinds of applications.

We know from physics that atoms are constantly moving; they move faster at higher temperatures, and slower at lower temperatures. This is why graphene and other two-dimensional materials cannot be completely flat and smooth. Even if thermal motion stopped completely (by cooling to absolute zero, 0 degrees Kelvin), atoms would still not remain at the same position. This is because of quantum mechanics, which says that even at the lowest temperature, the atoms would still perform some movement, known as zero-point motion. This quantum zero-point motion also creates ripples on graphene, and there is no way to stop it. Physicists would like to know the properties of these quantum ripples in

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graphene. They are however very hard to calculate, since quantum ripples are more complicated than thermal ones. And that is where the AUREL supercomputer steps in to help.

In 2013 Juraj Hašík, student of theoretical physics at the Faculty of Mathematics, Physics and Informatics of Comenius University in Bratislava, started to tackle the problem under the supervision of Prof. Roman Martoňák. He wrote a code that can simulate quantum ripples in graphene mathematically. However the quantum world is complicated, and the computation needs to perform a huge number of mathematical operations. If it were run on a standard personal computer, it would take many years. Thankfully Aurel is a parallel computer and can perform many (tens, hundreds, even thousands) computations at the same time. A big problem is split into small parts which can be solved separately and the whole is solved much faster. Writing such a program is not easy of course, but it is worth the effort. Juraj Hašík continued his research after he left to join a PhD programme at the International School for Advanced Studies, Trieste, Italy, where he also worked with Prof. Erio Tosatti.

What did AUREL tell us about the quantum ripples in graphene? It turned out that they are completely different from the classical ones. On longer distances they are weaker, and so graphene stays flat. On shorter distances they are stronger, making graphene more rough. Simply put, quantum graphene at lower temperatures is both flatter and rougher than the classical one. This work was published in the journal *Physical Review B* (04/04/2018) and the paper was also highlighted by the editors as the Editors' suggestion.

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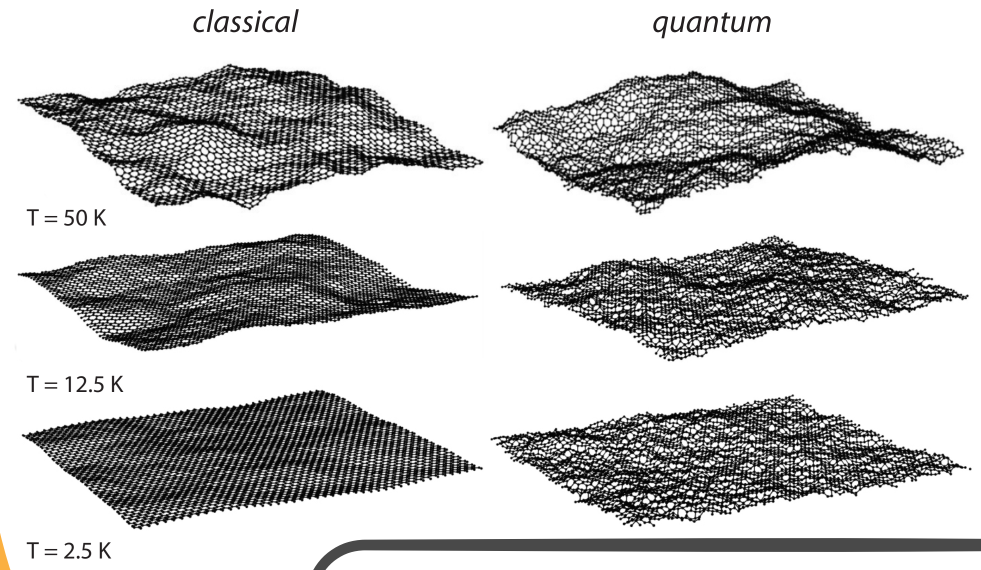

Rippled graphene from classical (left) and quantum (right) simulations at temperature 50 K (top), 12.5 K (center) and 2.5 K (bottom). Displacements in the vertical direction are amplified tenfold for better visualization.

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