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Sticky electrons: When repulsion turns into attraction

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Patrick Chalupa, Matthias Reitner, Alessandro Toschi (v.l.n.r.). Credit: Vienna University of Technology

Materials can assume completely different properties depending on temperature, pressure, electrical voltage or other physical quantities. In theoretical solid-state physics, state-of-the-art computer models are used to understand these properties in detail. Sometimes this works well, but sometimes strange effects occur that still seem puzzling—such as phenomena linked to high-temperature superconductivity.

A few years ago, scientists at TU Wien were already able to clarify mathematically where the boundary lies between the area that follows the known rules and the area where unusual effects play an important role. Now, with the help of complex calculations on supercomputers, it has been possible for the first time to explain exactly what happens when this boundary is crossed: The repulsion between the electrons is suddenly counteracted by an additional attractive force that enables completely counterintuitive effects.

Similar to the way water molecules combine to form droplets, the electrons can then come together at certain points, as if they were partially sticking together. The results, which were obtained in an international cooperation between TU Wien, the University of Würzburg, the University of L'Aquila and Georgetown University in Washington D.C., have now been published in the journal *Physical Review Letters*.

To infinity—and beyond

"Electrons are negatively charged, they repel each other. Therefore, electrons that move through the material are scattered by other electrons," says Prof. Alessandro Toschi from the Institute of Solid State Physics at TU Wien. "However, this scattering is not always equally strong. It is possible that the repulsion between the electrons is screened in the material. This depends on many factors, such as the chemical composition of the material."

Exactly at the borderline where unusual effects start to appear, the scattering processes between the electrons become theoretically infinitely strong due to the lack of screening. This is known as "divergence"—and these divergences pose a great challenge for research.

"For a long time, there was a very controversial discussion: Do these divergences actually have a real physical meaning?" says Patrick Chalupa, who is researching this problem as part of his dissertation in Alessandro Toschi's group. "We were able to answer this question: Yes, these divergences are not just a mathematical curiosity, but the key to a better understanding of important material effects," says Matthias Reitner, who wrote his Master thesis on this topic.

If you approach the mathematical limit, the repulsion becomes stronger and stronger. At the limit, the corresponding scattering between the electrons become infinitely large, but if you cross the limit, something surprising happens: The repulsion suddenly causes an additional attraction. This effective attraction forces the electrons to gather at certain points in a confined space, as if they were partially sticking together. This drastic change in behavior is closely related to the occurrence of the divergences.

Phase transition, similar to water vapor

"The result is a situation that is reminiscent of liquid water and water vapor," says Alessandro Toschi, "under certain conditions there is an attraction between the water molecules. They bind together and create a mixture of liquid droplets and gaseous steam. However, the origin of this attraction is completely different in the two cases."

For the first time, it has been possible to obtain a detailed picture of what happens in such situations from a materials science perspective on a microscopic level. "This means that it is now possible to understand exactly why certain mathematical approaches, so-called perturbative methods, did not produce the right result," says Patrick Chalupa.

This new microscopic insight could be a missing piece of the puzzle for the theoretical understanding of so-called unconventional superconductors. These are materials based on iron, copper or nickel that can be superconducting under certain conditions up to amazingly high temperatures. "Perhaps we will finally be able to answer some of the essential questions that have remained unanswered since the discovery of these mysterious materials 40 years ago," hopes Matthias Reitner.

More information: M. Reitner et al. Attractive Effect of a Strong Electronic Repulsion: The Physics of Vertex Divergences, *Physical Review Letters* (2020). DOI: 10.1103/PhysRevLett.125.196403

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