Change of perspective in the electronic landscape

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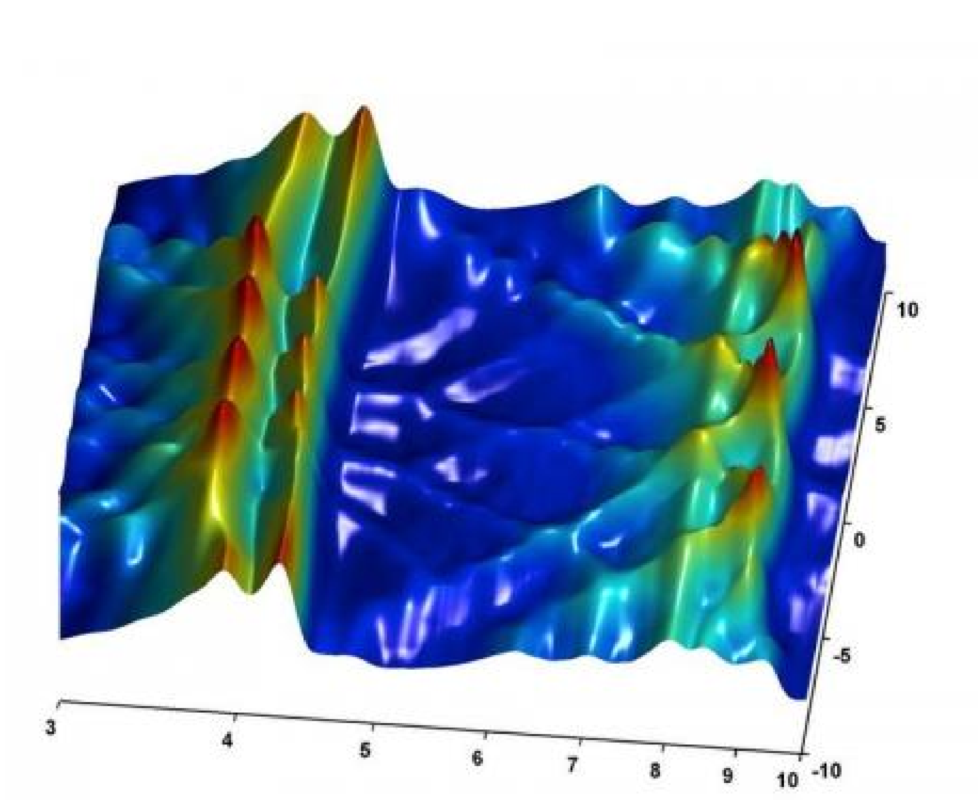


Electronic mountain range in the bismuth crystal: The relief map shows the energy distribution of the electrons as a function of the strength of the magnetic field in Tesla (T) and the tilt angle of the sample. Credit: MPI for Chemical Physics of Solids

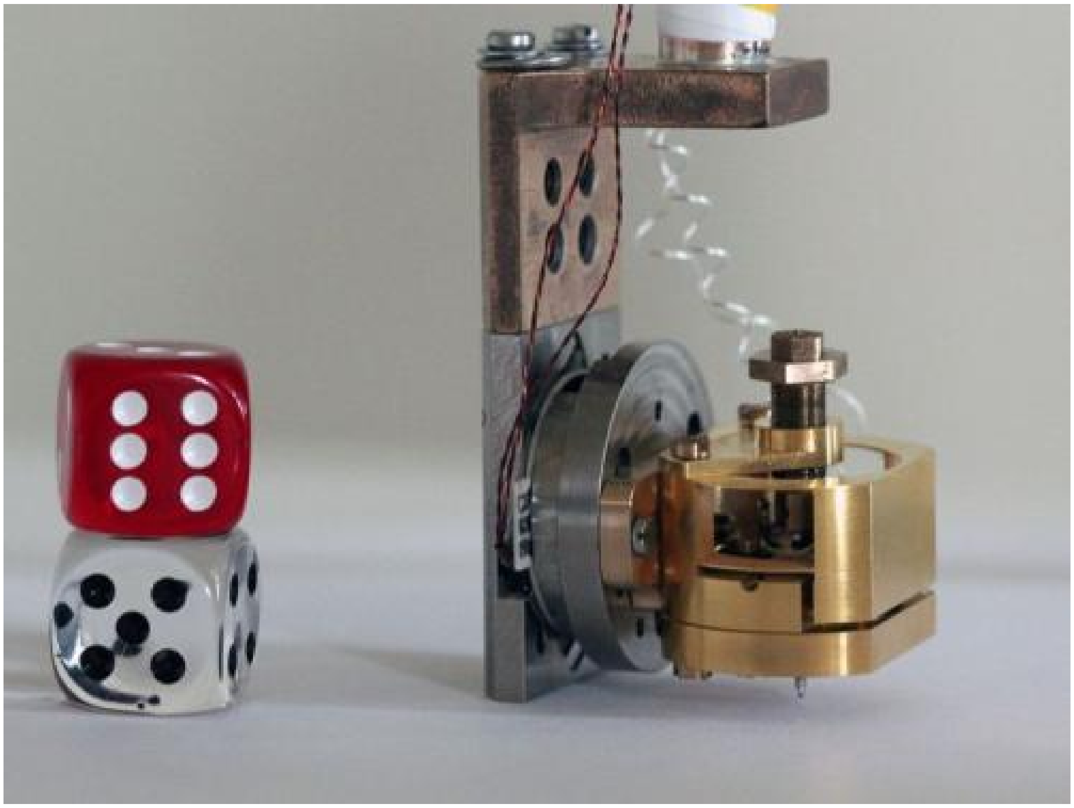
Time and again, even simple materials take physicists by surprise. Researchers at the Max Planck Institute for Chemical Physics of Solids in Dresden have observed an electronic property in the metal bismuth which they expected only in significantly more complex materials. In bismuth, electrons behave differently to free electrons in simple metals: depending on the direction in which they move through the crystal, it is sometimes easier and sometimes more difficult for them to make headway, as their energy distribution depends on the perspective. This can be compared to a mountain range where a hiker must surmount many high peaks on one route, but encounters only very few peaks on a different one. Remaining with this analogy, other metals resemble more a plain that looks the same in all three directions. In bismuth, the energy mountain range contains three so-called valleys in which the electrons can collect. Surprisingly, the electrons distribute themselves unevenly among these valleys of equal energy. The scientists discovered the unusual energy distribution using a very sensitive device which they had developed themselves for measuring the elongation of a sample. This method could also be used to investigate the electronic energy distribution in materials that are interesting for a completely new type of electronics.

Length, width and height can tell physicists more about a material sample than just its dimensions, because when the state of a substance changes, this also affects the arrangement of its components. This is very obvious when water freezes or evaporates: in one case, its molecules arrange themselves in a rigid lattice; in the other, they volatilize as a gas. Of course, this also changes the volume.

With other changes of state – physicists call them phase transitions – a material remains solid, but its crystal structure expands or contracts when an external magnetic field magnetises the substance, for example. The change in the sample dimensions is almost undetectable, however, when these transitions are investigated at a temperature of nearly absolute zero, i.e. at approx. minus 273 degrees Celsius. This is precisely the temperature range in which the physicists at the Max Planck Institute for Chemical Physics of Solids usually work, because many of the phenomena they are interested in occur only at these low temperatures. In order to measure how much a crystal expands or shrinks under these conditions, physicists require a very sensitive measuring device – and this is exactly what Robert Küchler has developed in his work at the Max Planck Institute for Chemical Physics of Solids. A Franco-German Team in this specific Project headed by Robert Küchler, Lucia Steinke and Kamran Behnia, who conducts Research at the ESPCI in Paris has now used this device and observed something about the metal bismuth that has taken the researchers pretty much by surprise.

A detailed image of the electronic energy distribution

The physicists applied a magnetic field to a bismuth crystal with a footprint of two millimetres by eight millimetres in different directions and slowly increased it. When the magnetic field strength increases, the electrons responsible for the charge transport rearrange themselves. This causes the volume of the metal to change slightly, and the sample expands or contracts in turn.



Measuring instrument for extreme dimensions: The thermal expansion cell enables researchers to measure changes in length of approximately one thousandth of a nanometre, i.e. one billionth of a millimetre, at temperatures between room temperature and minus 273.1 degrees Celsius. A sample is clamped between the two plates of a capacitor whose capacitance changes when the sample expands or contracts. This change in capacitance can be measured very accurately by the change in a voltage. The scientists can thus detect changes in length which are one hundred times smaller than the separations of the atoms in the crystal lattice. Credit: © MPI for Chemical Physics of Solids

The researchers determined the tiny changes in length for the various orientations of the magnetic field with an extremely sensitive dilatometer, which measures the expansion of a sample. From the sample's change in length they deduced the changes in the electronic distribution in the respective direction of the magnetic field and used this information to draw a type of relief map. Physicists refer to this as determining the energy distribution or energy structure of the electrons as a function of the magnetic field. "We've measured this relief map for bismuth, which shows how the electronic structure changes as a function of the magnetic field, more precisely than has been possible to date using other methods," says Robert Küchler.

The energy structure in bismuth has three identical minima, so-called valleys, in which the electrons can collect. The electrons similarly distribute themselves over different valleys in other materials as well, such as the semiconductor silicon. This energy distribution of the electrons manifests itself in precisely those properties which make the material so interesting for the semiconductor industry.

In a pure bismuth crystal, physicists would expect to find equal numbers of electrons in the valleys of equal energy, as is the case in silicon. "But, surprisingly, the electrons in bismuth do not distribute themselves completely uniformly over the three valleys," explains Lucia Steinke. "At specific magnetic fields, the valleys are filled or emptied differently, resulting in clear asymmetries in the relief map."

Bismuth electrons sense each other more strongly than is usual in metals

Physicists actually expect electrons in apparently identical valleys to behave differently in more complex materials such as ceramics, which are structured like a layer cake. At the moment, the researchers in Dresden cannot ultimately explain why bismuth also behaves in this way. However, they already have a suspicion. The electrons of bismuth possibly interact much more strongly with each other than the charge carriers of conventional metals. This would mean that the idea which physicists have of the electronic order in metals would no longer apply to bismuth.

The researchers and principal authors of the current study and their most important instruments: Robert Küchler (right) mounting the bismuth crystal in the measuring cell and Lucia Steinke using her laptop to evaluate the data. Credit: MPI for Chemical Physics of Solids

The conventional model considers the electrons which provide shine and electricity transport in metals as a lake. The lake of these conduction electrons washes around the atomic cores. With this idea, each individual electron sees only one electrostatic field which results from averaging over the other negative charge carriers in the lake and the positively charged atomic cores. "It would seem that this approximate description does not apply to bismuth, because some of its electrons sense each other more strongly than the model of metals predicts," says Robert Küchler. Here as well, the metal is more similar to more complex materials such as some ceramics.

Novel electronics could exploit the electronic energy distribution

The discovery of the unusual properties of bismuth electrons is not the only insight which Robert Küchler and his colleagues have gained in their work, however. "We showed that our very sensitive dilatometer is also suitable for investigating the electronic structure of materials," says Robert Küchler, who is meanwhile also marketing the precision instrument in a spin-off company. One application is to investigate the electronic energy distribution in materials where the distribution of the electrons among the valleys changes with the perspective, just like in bismuth, but can also be manipulated arbitrarily. Such materials could be interesting for a completely new type of electronics: valleytronics, from the words valley and electronics.

In valleytronics, the 0 and 1 of a data bit could be assigned to two different distributions of the electrons among the valleys. Computations would then involve the electrons being shifted to and fro between different valleys. What makes the electronic valleys so special as a computing tool is that they can serve as quantum bits from which superposition states can be generated. These mixed states of two or more valleys make it possible to execute significantly more computing operations in one step than is possible with the normal computers available today. A quantum computer that operates like this would therefore be much faster than a conventional one for some tasks. But it will certainly be a while yet before this is the case. The exceptionally precise dilatometer designed by the Dresden-based scientists and their research on materials with unusual electronic properties could help to overcome a few obstacles on the road to valleytronics, however.

More information: Robert Küchler, Lucia Steinke, Ramzy Daou, Manuel Brando, Kamran Behnia and Frank Steglich. "Thermodynamic

evidence for valley-dependent density of states in bulk bismuth." *Nature Materials*, Mai 2014; [DOI: 10.1038/nmat3909]

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