The metal-insulator transition depends on the mass of the Dirac electrons

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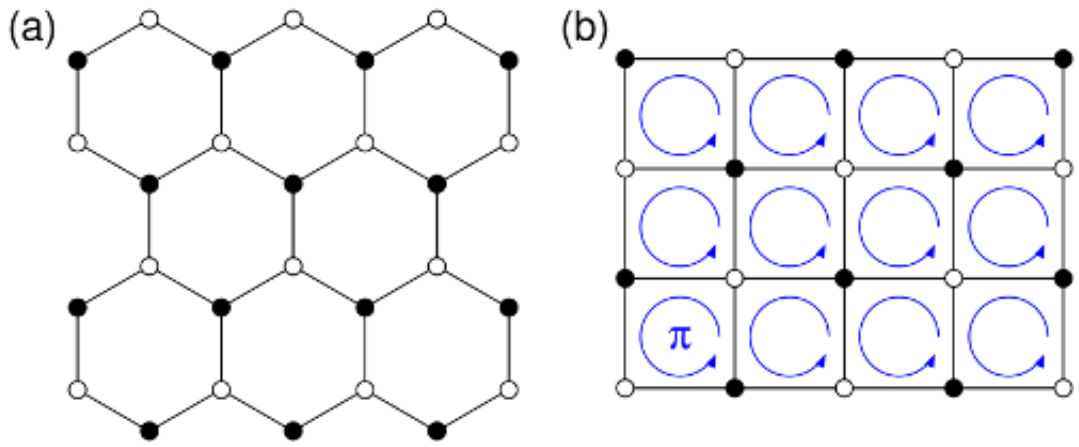


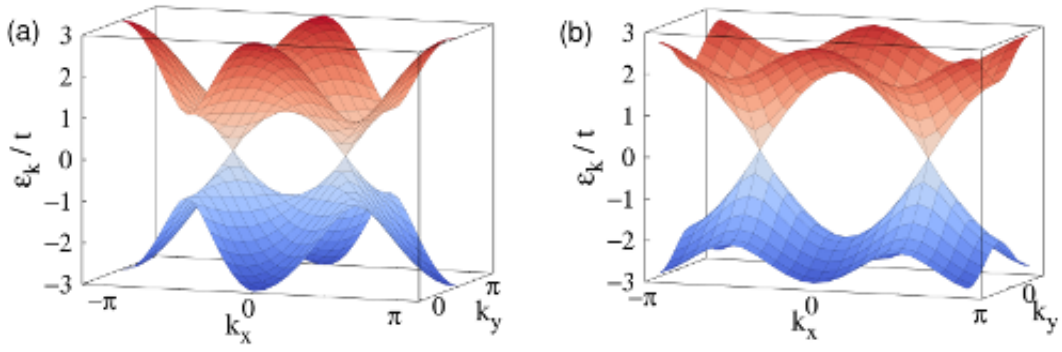
Structure of a honeycomb (left) and pi-flux (right) lattice

Scientists from the RIKEN Advanced Institute for Computational Science (AICS) in Kobe, Japan, have used the powerful K computer, along with a number of other supercomputers, to perform a large-scale analysis of the behavior of electrons in a material transitioning from a metal to an insulator phase. Their analysis, just published in *Physical Review X*, confirmed that there is a direct movement between the two phases, and that the behavior is tied to the loss of mass of the electrons—called Dirac electrons—in the materials as they become correlated with one another.

Most materials maintain a certain property—either conducting or

insulating—consistently, but there are a class of materials that can transition from one state to another based either on environmental changes, such as pressure or magnetic field, or by "doping" with other materials. How this happens has long been a mystery. Hints came from the fact that "band theory"—which explains the properties of materials by looking at the bands occupied by electrons and the difficulties of jumping from one to another—gave wrong predictions for certain classes of materials. Nevill Mott, in work that earned him the 1977 Nobel Prize in Physics, came to understand that this inaccuracy was due to the correlation between electrons in these materials, which are affected by the repulsive Coulomb interactions between them.

To shed new light on this problem, the team began modeling large numbers of electrons on two lattices with about 100 to 3,000 sites, using variations of the Hubbard model, which has been successful in modeling such materials. They found that, in contradiction to theories that there was a transitional phase, there was in fact a direct transition from metal to insulator as the correlation between the electrons increased, and the use of the large-scale simulation enabled them to determine, with new accuracy, when the transition would take place. They discovered also that the key element was the loss of mass of the Dirac electrons, not the speed at which they traveled, which seemed unrelated to the transition.



Noninteracting energy dispersions in the honeycomb (left) and pi-flux (right)

The authors also discussed the fact that this metal-insulator transition, expected to arise in graphene-like materials, can be understood in terms of the language of particle physics, despite the fact that the electrons in the graphene and the elementary particles such as quarks dealt with in particle physics have totally different energy scales. According to this language, the transition they elucidated corresponds to the breaking of the so-called chiral-Heisenberg symmetry in the celebrated Gross-Neveu model introduced more than 40 years ago.

According to Yuichi Otsuka, the first author of the work, "Our study determines for the first time the universality class of the metal-insulator transition of interacting Dirac electrons. We expect that our findings will be relevant not only to condensed matter materials but also to Dirac fermions in particle physics." He continued, "There are still many things we do not understand about interaction-driven insulators, and research in this area may help us elucidate those mysteries."

More information: Yuichi Otsuka et al. Universal Quantum Criticality in the Metal-Insulator Transition of Two-Dimensional Interacting Dirac Electrons, *Physical Review X* (2016). DOI: 10.1103/PhysRevX.6.011029

Provided by RIKEN