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Coupled electrons and phonons predicted to flow like water in 2D semiconductors

A condition long considered to be unfavorable to electrical conduction in semiconductor materials may actually be beneficial in 2D semiconductors, according to new findings by UC Santa Barbara researchers published in the journal Physical Review Letters.

Electron-phonon interactions — collisions between charge-carrying electrons and heat-carrying vibrations in the atomic lattice of the material — are considered the primary cause of electrons slowing down as they travel through semiconductor material. But according to UCSB mechanical engineers Bolin Liao and Yujie Quan, when electrons and phonons are considered as a single system, these interactions in atomically thin material prove to actually conserve total momentum and energy, and could have important implications for 2D semiconductor design.

“This is in sharp contrast to three-dimensional systems where you have a lot of momentum loss processes,” said Liao, who specializes in thermal and energy science.

Diffusion and hydrodynamic flow

There are two main types of energy transport that underlie the researchers' concept: hydrodynamic flow, a collective kinetic process where the individual components of a fluid move together in a general direction, like water flow in a pipe; and diffusion, in which particles undergo random walks driven by a gradient of concentration or temperature, like smoke. Typically heat conduction in solids is understood to be a diffusion process.

"These are two very different physical processes," Liao said. In the case of hydrodynamic flow, which is more efficient in transporting energy than diffusion, the total momentum of particles is conserved during their collision processes. Though they can collide with each other they exchange their momentum and continue to move together.

"But when we think of heat conduction in material, it is not carried by 'real' particles," Liao continued. Rather, phonons, which we can think of as "heat particles," are the result of collective vibrations of the material's atoms, and they tend to diffuse, with microscopic collisions that don't conserve momentum — a less efficient process for transporting energy. It's the interactions between phonons and electrons that cause electrons to slow down, or their momentum to relax. It's the reason why electrical resistance of conductors decreases at a lower temperature — the lack of thermal energy diminishes the resistance electrons would encounter in the material.

However, according to Liao and Quan, the physics is different in two dimensions. "They have some unusual properties," Liao said of atomically thin semiconductors. "For example, in these materials, such as graphene, when the phonons scatter with each other, it is known that their momentum is largely conserved. This is due to the different dimensionality that imposes some constraint on how they can interact with each other."

In their simulations of 2D semiconductors with strong electron-phonon interactions, the researchers found that when treating both the charge and heat carriers as part of the same system, the interactions between electrons and phonons resulted in a collective hydrodynamic flow behavior.

"They start to move together like molecules in a fluid flow," Liao said. "They drift together with the same velocity, like fluid flow through a pipe." This process, so-called "coupled electron-phonon hydrodynamics," reflects how this combined system flows like a classical liquid. In this process, Liao said, fluid flow, heat diffusion and even electric conduction “can become very similar.”

“We can show that if you take into account this hydrodynamic behavior, the charge transport on two-dimensional material can be very efficient,” he explained, “much more efficient than people would expect from just looking at how frequently they collide with the heat carriers.”

These findings have important implications for 2D semiconductor design, and the potential for achieving highly efficient electrical conductivity even at room temperature. While one way to encourage such efficiency would be to lower temperatures to reduce collisions, Liao said, “our new idea here is instead of trying to reduce how often they collide, we can just engineer the material to make sure most of the collision processes are momentum-conserving.” So while charge carriers could still lose some momentum to collisions with heat particles, the system’s total momentum conservation will ultimately result in low dissipation and highly efficient transport.

In their paper the researchers prove their concept with an investigation of atomically-thin molybdenum disulfide (MoS_2), finding that charge mobility can be enhanced by almost seven times when taking into account hydrodynamic behavior.

“That’s a very significant enhancement,” Liao said. In addition to providing a more practical alternative to ultra-low temperature superconductivity, focusing instead on the material’s ability to host hydrodynamic electron-phonon behaviors “can be very promising for microelectronic applications.”

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