Speeding up calculations that reveal how electrons interact in materials

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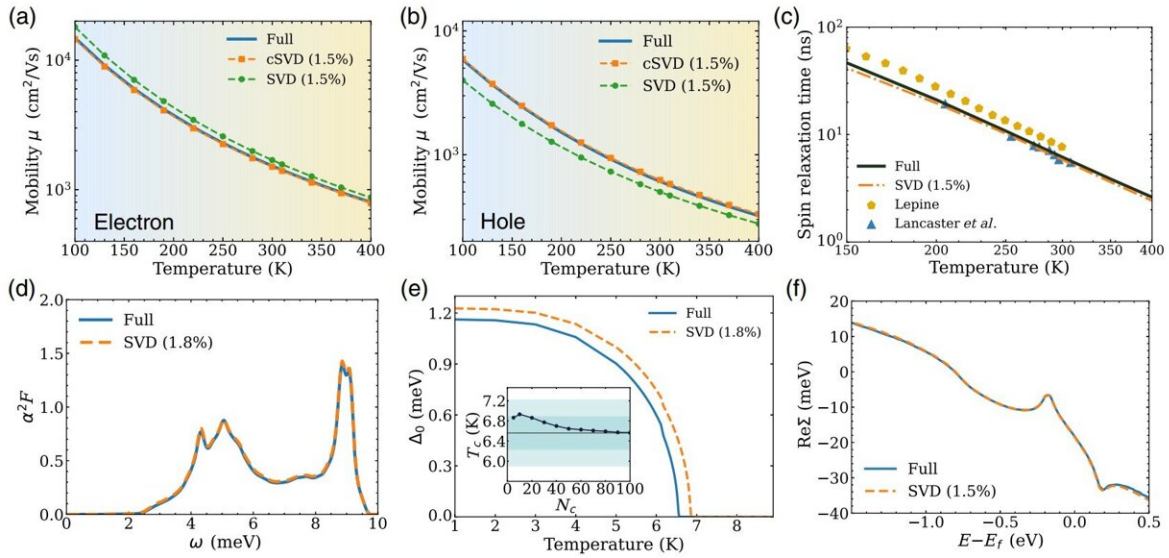

Credit: *Physical Review X* (2024). DOI: 10.1103/PhysRevX.14.021023

Materials scientists and engineers would like to know precisely how electrons interact and move in new materials and how the devices made with them will behave. Will the electrical current flow easily within the material? Is there a temperature at which the material will become superconducting, enabling current to flow without a power source? How long will the quantum state of an electron spin be preserved in new electronic and quantum devices?

A community of materials physicists attempt to address such questions by understanding what takes place inside materials, calculating their behavior down to the level of individual electron interactions and atomic motions.

Now a Caltech team has made a key discovery that helps simplify such calculations, speeding them up by a factor of 50 or more while maintaining accuracy. As a result, it is possible to compute electron interactions in more complex materials and devices as well as to develop new calculations that were previously thought impossible.

In a new paper published in the journal *Physical Review X*, Caltech's Yao Luo, a graduate student in applied physics; his advisor Marco Bernardi, professor of applied physics, physics and materials science; and colleagues describe a new data-driven method that has enabled these advances. Their approach simplifies the dense computational matrices used to represent the interactions that take place in a material between electrons and atomic vibrations (or phonons, which can be thought of as individual units of vibrational energy).

Luo and Bernardi say that the new method allows them to use only 1 to 2% of the data typically used to solve such problems, greatly accelerating calculations and, in the process, revealing the most important interactions that dictate the properties of materials.

"This was very surprising," says Bernardi. "The electron–phonon interactions computed with the compressed matrices are nearly as accurate as the full calculation. This reduces the computing time and memory usage tremendously, by about two orders of magnitude in most cases. It's also an elegant example of Occam's razor, the idea of favoring simple physical models with minimal numbers of parameters."

Finding a new middle ground for the field

Researchers in this field generally follow one of two approaches to understand materials on this most fundamental level. One approach emphasizes building minimal models, reducing the complexity of the system, so that researchers can tweak a handful of parameters in pen-and-paper calculations to get a qualitative understanding of materials.

The other begins with nothing more than the structure of a material and uses so-called "first principles" methods—quantum mechanical calculations requiring large computers—to study materials properties with quantitative accuracy.

This latter set of methods, which Bernardi's group focuses on, use extremely large matrices featuring billions of entries to compute electron interactions that control a wide range of physical properties. That translates to thousands of hours of computing time for each calculation. The new work suggests a kind of middle ground between the two approaches, Bernardi says.

"With our new method you can truncate the size of these matrices, extract the key information, and generate minimal models of the interactions in materials."

Rooting out the most important singular values

His group's approach is based on applying a method called singular value decomposition (SVD) to the electron–phonon interactions in a material. The SVD technique is widely used in fields like image compression and quantum information science. Here, it allows the authors to separate, or disentangle, the electronic and vibrational components in a matrix of thousands or millions of electron–phonon interactions and to assign each fundamental interaction a number.

These real positive numbers are called singular values and rank the fundamental interactions in order of importance. Then the program can eliminate all but a few percent of the interactions in each matrix, leaving only the leading singular values, a process that makes the determination cheaper by a factor proportional to the amount of compression.

So, for example, if the program keeps only 1% of the singular values, the calculation becomes faster by a factor of 100. The researchers have found that keeping only a small fraction of singular values, typically 1 to 2%, the approximate result retains nearly the same accuracy as the full calculation.

"By using SVD, you can cut the number of singular values and capture only the main features of the matrices representing electronic interactions in a given material," says Luo, lead author on the paper who is in his third year in Bernardi's group.

"This truncates the original matrix, thus speeding up the algorithm, and has the added benefit of revealing which interactions in the material are dominant."

Bernardi notes that this latter benefit of the SVD method gives the researchers a "physical intuition" about electron interactions in a material, something that has been missing from the first principles calculations in the past. For example, in a calculation involving silicon, it became clear that the dominant singular value was associated with the stretching and squeezing of a particular bond.

"It's something simple, but before doing the calculation, we didn't know that was the strongest interaction," explains Bernardi.

In the paper, the researchers show that the compression of matrices related to electron–phonon interactions using the SVD method provides

accurate results for various properties of materials researchers might want to calculate, including charge transport, spin relaxation times, and the transition temperature of superconductors.

Bernardi and his team are extending the SVD-based calculations to a wider range of interactions in materials and developing advanced calculations that were previously thought impossible. The team is also working to add the new SVD method into its open source Perturbo code, a software package that helps researchers calculate how electrons interact and move in materials. Bernardi says that this will enable users in the scientific community to predict material properties associated with electron–phonon interactions significantly faster.

The paper is titled "Data-driven compression of electron-phonon interactions." Along with Luo and Bernardi, co-authors on the paper include graduate student Dhruv Desai (MS '22); Benjamin Chang (MS '20), and Jinsoo Park (Ph.D. '22), who is now a postdoctoral fellow at the University of Chicago.

More information: Yao Luo et al, Data-Driven Compression of Electron-Phonon Interactions, *Physical Review X* (2024). DOI: 10.1103/PhysRevX.14.021023

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