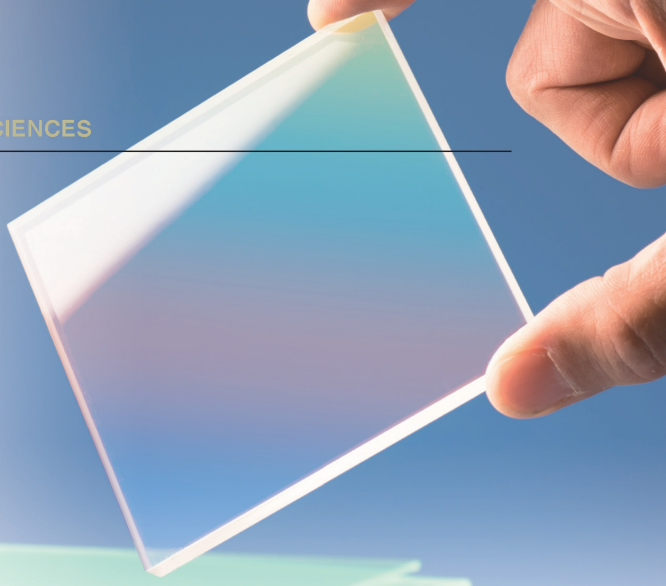

Fast band structure computation using a new and efficient hHybrid method

Imagine you are an Uber driver and happen to pick up a material scientist or a physicist. What would be the first question you asked her/him? I could give the reader some examples based on my personal experience. This approach may seem naive or biased, but such questions may lead brilliant minds to dedicate themselves to the field. Two frequently asked questions are (i) how do people distinguish different phases of matter and (ii) what are the main challenges in material science?

Of course, these questions cannot be fully answered. Instead, I will try to narrow them down in the following paragraphs and relate them to the work that will be introduced.

First, I address question (i). The physics of phase transition includes dozens of branches. One of the most practical branches is the study of insulators and conductors, which seeks to determine if a given material is insulating or conducting. At the level of single-electron physics, physicists have acquired considerable knowledge about this question since the 1930s. If an electron is placed in a periodic array formed by ions, the energy of the electron will form energy bands. According to how electrons fill the energy bands and the energy difference between the highest occupied and lowest unoccupied bands, one can roughly determine if a material is insulating or conducting. In the 21st century, we can engineer exotic band structures. For example, we can place photons, or electromagnetic waves, in a periodically stacked dielectric/metal array. Applying similar ideas ranging from ordinary crystals to the Maxwell equations, scientists now can build “photonic crystals” and study their band structures.

The natural question that follows is how the band structure of a photonic crystal model is determined? Due to developments in computational science, many continuum problems can now be properly discretized and formulated in terms of matrix diagonalization problems, which is my short response to question (ii).

From a computational perspective, one of the greatest challenges is our limited ability to diagonalize a given matrix. Some readers might have learned matrix algebra in various contexts and likely found it tedious, except when the matrices are diagonal. This finding is true even in advanced studies. Additionally, some methods can be effectively applied for some particular problems. Nonetheless, given a general large matrix, no numerical approach exists that can efficiently diagonalizes the matrix or even determine some of the smallest diagonal entries or eigenvalues.

In a recent work, Huang, Lin, and Wang studied the band structure of a particular dispersive metallic photonic crystal based on the three-dimensional lossless Drude model with a face-centered cubic (FCC) lattice. They reformulated the non-linear problem in terms of standard eigenvalue problems that were “easier” to numerically solve.

However, such problems remain far from easy to solve. In turn, they pointed out the numerical challenge involved in determining the solution, including reasons that conventional and popular approaches may not consider. Such problems are inhibited by the following three factors: (a) the high multiplicity of zero eigenvalues; (b) the desired eigenvalues are clustered, which means the eigenvalues of interest have extremely small spacings; and (c) the lack of an efficient preconditioner. The first issue prevents the solvers from operating efficiently. The second issue affects the error bounds of the computation. The third issue requires some more elaboration. In numerical linear algebra, many

approaches involve iterations of matrix operations. If one starts from a "reasonable" initial value, or preconditioner, the computation converges significantly faster.

To tackle these problems, various methods of performing similar computations, such as the "SI-Lanczos" and variants of "Jacobi-Davidson" methods, e.g., "sJD", "hJD", "hSIRA", etc. The strong and weak features of these approaches have been analyzed and discussed to identify potential solutions to the aforementioned three problems. As such, a new variant method, "hHybrid", was developed. This method features (a) harmonic Rayleigh-Ritz extraction, (b) hybrid usage of "sJD" and "hSIRA", and (c) a fast Fourier transform-based preconditioner. Each feature can solve the corresponding problems (a)-(c).

Intensive computations for multiple test problems were implemented, and the results demonstrated that the "hHybrid" method outperformed other existing methods in terms of computational efficiency. Additionally, some plausible research directions and potential extensions to the "hHybrid" method were proposed.

In summary, a new numerical scheme was recently proposed for the computation of a certain class of photonic crystal band structures. In numerical experiments, it outperformed other common methods. In the opinion of the author, it not only provides with new insights for experts in the field but also helps move toward the ultimate grand questions asked at the beginning of this article.

Reference

Huang, T., Lin, W., and Wang, W. (2016). A hybrid Jacobi–Davidson method for interior cluster eigenvalues with large null-space in three dimensional lossless Drude dispersive metallic photonic crystals. *Computer Physics Communications, 207*, 221-231. DOI:10.1016/j.cpc.2016.06.017

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Contribution of the thermal Hall effect to the anomalous Nernst and spin Seebeck effects

Heat dissipation has been the most formidable challenge in information technology due to the continued increase in power dissipation, and it has hampered the development of charged-based electronic devices. Unlike purely charge-based systems, information devices encoded in magnetization states in spintronics are nonvolatile, which can reduce the power requirement for maintaining the data. Therefore, within a very short period of time, we have witnessed the remarkable success of spintronics to transfer fundamental science into practical applications.

The manipulation of the spin-dependent transport properties in terms of the spin-polarized current ($\boldsymbol{J}_{SP}$) or pure spin current ($\boldsymbol{J}_{S}$) is one key aspect in the field of spintronics. The anomalous Nernst effect (ANE) and the spin Seebeck effect (SSE) are two of the most important mechanisms that generate and detect the $\boldsymbol{J}_{SP}$ and $\boldsymbol{J}_{S}$ by thermal excitation, respectively. Thus, research regarding the interplay among the charge, spin, and heat in the ANE and SSE has been intensively conducted. Nevertheless, recent research suggests that the thermal Hall effect (THE) has field dependences that are indistinguishable from, and may even overwhelm, those of the ANE and SSE. Therefore, it is vital to investigate the contribution of the THE in the ANE and SSE. In this work, for the first time, we suc-