Wannier90 v3.0 school, Virtual Edition 2020

Speaker: Roxana Margine

27 March 2020 - Questions and answers session

- **What do you mean by virtual phonons? [Slide 15]**
    - The notion of virtual particles appears in perturbation theory. A virtual phonon is a mathematical term that appears in the perturbative expansion of interactions involving phonons.
    - In the top right figure on Slide 15, an electron emits a virtual phonon, and this phonon is absorbed by another electron. This results in an *effective electron-electron interaction*. The emission of virtual phonons by electrons means a deformation (polarization) of the lattice in the vicinity of the electron (as shown in the top left figure on Slide 15). If a second electron is near this polarization cloud, the two electrons become correlated and form a Cooper pair.
- **Prediction of energy gap is not a delicate issue in the DFT calculations? [slide 16]**
    - The discussion on superconductivity is about metals not semiconductors.
- **What software did you use to create the beautiful color plot of BZ in page 20?**
    - There is a YouTube video to explain how to do such a plot. You can find it at https://www.youtube.com/watch?v=7jZ-C5FNfgU
- **How to calculate the Coulomb pseudopotential?**
    - One can for example use the SterheimerGW code. You can see a discussion on this topic in the following reference: C. Heil, S. Ponce, H. Lambert, M. Schlipf, E. R. Margine, and F. Giustino, Phys. Rev. Lett., 119, 087003 (2017) https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.119.087003
- **How did you deal with charge density wave in NbS2 calculations? I think some of NbS2 mode is imaginary related to CDW phase in this type of material. I mean how to incorporate CDW contribution to el-ph interaction if CDW and superconductivity co-exist in some material.**
    - In NbS2, quantum anharmonic effects remove the instability found at the harmonic level both in bulk and monolayer. This is discussed in the following studies: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.119.087003 https://pubs.acs.org/doi/10.1021/acs.nanolett.9b00504
      In general, one reconstructs the crystal structure following the eigenvector(s) of the CDW mode (i.e., the imaginary mode), and re-evaluates the e-ph interaction of the resulting structure.
- **I am wondering if it is possible to have Eliashberg in the real space only (you mentioned that there are less matrix element g(RR')).**

    - One will have to see if the Migdal-Eliashberg formalism can be written entirely in real space. I am aware of one study in which the superconducting order parameter was calculated in real space from the first principles density functional theory for superconductors (SCDFT). The reference is given below: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.115.097002
- **Why EPW cannot deal with eletron-phonon interactions in 2D?**
    - The long-range analytic part is different in 2D than in 3D. In the 2D case, one needs to truncate the Coulomb potential along the non-periodic direction. This implementation will be released soon in EPW.