Poster-2-34

WannierBerri code : berryology made fast and easy.

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Wannier interpolation is a powerful tool for performing Brillouin zone integrals over dense grids of k points, which are essential to evaluate such quantities as the intrinsic anomalous Hall conductivity, electron-phonon coupling strength or Boltzmann transport coefficients. This methodology was implemented in the well-known Wannier90 [1] and other related packages (EPW[2], WannierTools[3], etc).
However, with more complex physical problems and materials computations with the existing codes become very expensive, which often prevents reaching the desired accuracy. Over the years it was overlooked that some rather simple modifications of algorithms can boost the speed of Wannier interpolation by several orders of magnitude. They include a combination of fast and slow Fourier transforms, explicit use of symmetries, recursive adaptive grid refinement and tetrahedron integration among others. All those methods were implemented in a new python code WannierBerri [4].
Further, involving a broad collaboration of co-developers, we work on extending functionality. The philosophy of the code is to give the user a toolbox, where one can write a minimal code to construct the evaluation of a any new quantity from basic building blocks, such as band velocities, Berry curvature or Berry connections, orbital moment and others.

[1] http://www.wannier.org/ G. Pizzi et al, J. Phys.: Condens. Matter 32 165902 (2020).
[2] https://epw-code.org/ S. Poncé, E. R. Margine, C. Verdi, and F. Giustino, Comp. Phys. Commun. 209, 116 (2016).
[3] http://www.wanniertools.com/ Q. Wu, Sh. Zhang, H.-F. Song, M. Troyer, A.A. Soluyanov, Comp. Phys. Commun. 224, 405 (2018).
[4] https://wannier-berri.org/ Stepan S. Tsirkin, npj Comput Mater 7, 33 (2021).