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Soliton signature in the phonon spectrum of twisted bilayer graphene

The discovery of unconventional superconductivity in slightly-misaligned bilayer graphene [1] has triggered an important enthusiasm from the scientific community. While the electronic properties of such a system have already been carefully examined by the means of the theoretical approaches, its vibrational properties have yet to be fully-explored. In this work, we investigate the phonons for a set of 692 twisted bilayer graphene structures, combining force field and an unfolding scheme in order to unravel the numerous phonon modes of the considered systems. The emergence of phonon side bands at the high-symmetry points of the graphene Brillouin zone is highlighted, especially for small mislignement angles between the layers. Those side bands are rationnalized with the introduction of the Nearly-Free Phonon Model, which can be understood as the counterpart for phonons of the Nearly-Free Electron model [2], where the electrons and the nucleus potential have been respectively replaced by the phonons and the soliton network potential.

References

[1] Y. Cao, V. Fatemi *et al.*, Nature **556** (2018)
[2] K. M. Rabe, Physics Today **55**, (2002) 61

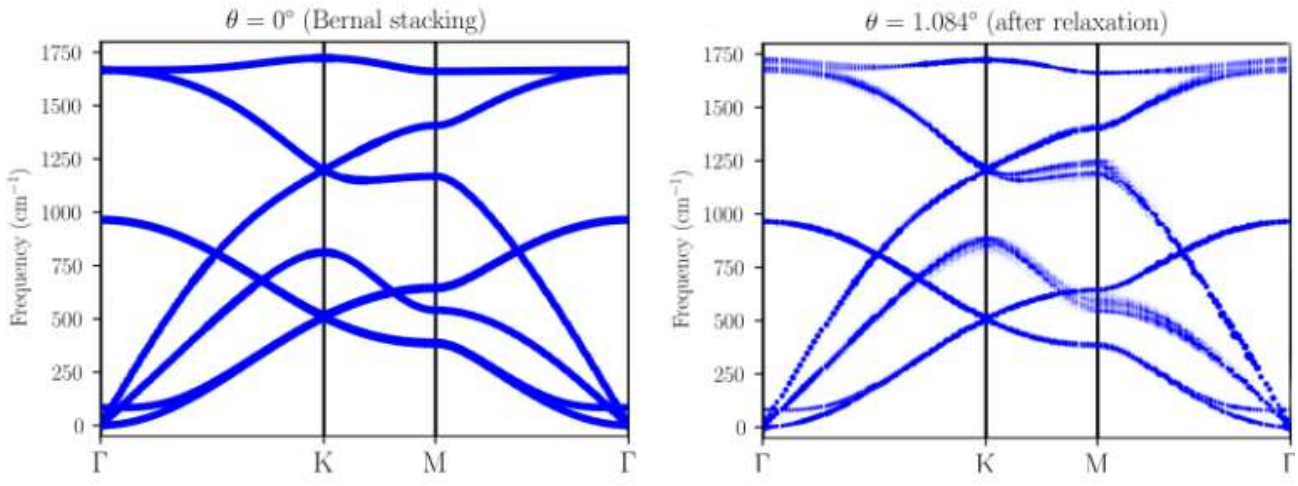

Figure 1: phonon band structure of (left) aligned bilayer graphene and of slightly-misaligned bilayer graphene (unfolded on the Brillouin zone of the graphene bottom layer). Side bands emerge at the high-symmetry points of the Brillouin zone.