O.28 Long-range dielectric screening and interatomic force constants in two dimensions

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The foundation of modern theory of lattice dynamics rests on the separation between short-range and long-range interatomic force constants, where the latter are associated with macroscopic electric fields acting in a neighborhood of the Brillouin zone center. In three-dimensional (3D) insulators, the famous dipole-dipole formula was established long ago by Cochran and Cowley; the subsequent work of Pick, Cohen and Martin provided a formal derivation in the framework of first-principles theory. Very recently, we have incorporated higher-order interactions involving, e.g., dynamical quadrupoles, and demonstrated their role in the accurate interpolation of phonon band structures. [1]

In this talk, I shall retrace an analogous journey in the context of two- dimensional (2D) crystals, by presenting a rigorous derivation of the long- range screening and interatomic forces in 2D. This enables a systematic generalization of the existing formulas (T. Sohier *et al.*, Nano Lett. 2017, 17, 6, 3758) to an arbitrary multipolar order. In particular, I will discuss how to incorporate out-of-plane dipoles and dynamical quadrupoles in the long-range part of the dynamical matrix, and how to achieve an optimal representation of the dielectric function. Numerical tests on monolayer BN, SnS_2 and $BaTiO_3$ membranes demonstrate a drastic improvement in the description of the long-range electrostatic interactions, with comparable benefits to the quality of the interpolated phonon frequencies. [2]

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[1] M. Royo, K. Hahn and M. Stengel, Physical Review Letters, **125**, 217602 (2020).

[2] M. Royo and M. Stengel, https://arxiv.org/abs/2012.07961