Mechanically stable graphene with quadratic out-of-plane acoustic modes

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The phonon properties of 2D materials are far from trivial as the harmonic approximation predicts fast diverging atomic displacements as a function of the sample size and finite linewidths of the longitudinal and transverse in-plane acoustic phonon modes at small momenta. These problems arise due to the quadratic dispersion of the acoustic out-of-plane phonon frequencies obtained in the harmonic approximation. By including anharmonicity within the self-consistent harmonic approximation (SCHA) we show that the divergences in the atomic displacements are suppressed and the linewidths of in-plane acoustic phonons vanish at low momenta, recovering the physical picture. By calculating the phonon spectra from the Hessian of the anharmonic free energy, we conclude that the physical dispersion expected experimentally for the acoustic out-of-plane mode should be quadratic (see Figure 1). We verify this result both using atomistic simulations and using a membrane model for graphene. Our conclusions [1] have a crucial role in the understanding of the mechanical and thermal properties of graphene and other strictly two-dimensional material.

References

[1] U. Aseginolaza *et al.* in preparation.

Figures

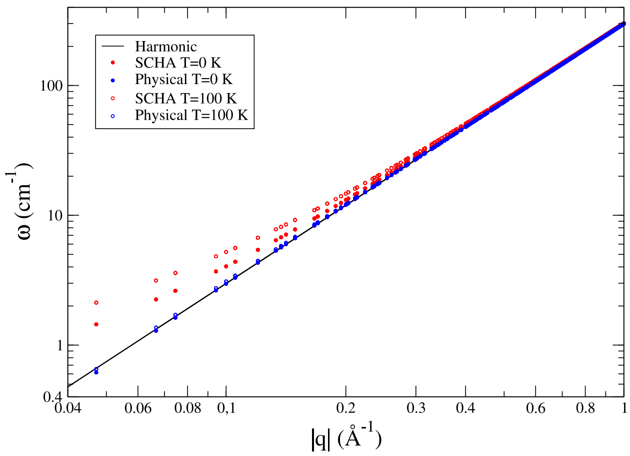

Figure 1: Frequency of the ZA mode in the harmonic approximation, within the SCHA and obtained from the Hessian of the SCHA (labeled as "Physical") both at 0 K and 100K using the membrane model. The physical phonons recover the quadratic dispersion of the harmonic solution.