TUNING INFRARED PHONON ANOMALIES IN OPTICAL CONDUCTIVITY OF BILAYER GRAPHENE: MATCHING THEORY AND EXPERIMENT

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The detection and analysis of the spectral properties of optical phonons in (single-layer and multilayer) graphene provides a powerful tool not only for investigating the role of the underlying electron-phonon interaction, but also for a careful characterization of the systems (charge doping, number of layers, stacking order, amount of disorder etc.). The large majority of the studies in this field have been performed so far by using Raman spectroscopy. Within this context, the investigation of phonon anomalies in the optical infrared (IR) spectra can shed a useful complementary light on the issue, due to the different selection rules. In pristine bilayer graphene, in particular, two nearly degenerate in-plane modes with characteristic frequency $\omega_0 \approx 0.2$ eV are expected to be relevant, the symmetric (E_g) and the antisymmetric (E_u) ones, active respectively in the Raman and in the IR spectra.

In this contribution, after reviewing the experimental findings, we present a unified microscopic theory, in terms of the charged-phonon effect, which permits to take into account in graphenes at the same level of the phonon intensity and the Fano asymmetry [3]. We show that these two features are strictly related stemming from the quantum interference between the electronic and phononis degrees of freedom. Within this context we are also able to elucidate the relative role of the E_u and E_g phonon modes in regards to the infrared activity and the Fano asymmetry of the observed phonon peaks. We present thus a complete phase diagram for the strength of the phonon modes and their Fano properties as functions of the chemical potential μ and of the gated-induced electronic Δ gap (Fig. 1), showing that a switching mechanism between the dominance of the E_u or E_g mode can be controlled by the external gate voltage. Our work permits thus reconciling within a unique approach the phonon-peak features observed by different experimental groups, and it provide a theoretical tool for predicting and controlling on a quantitative level the spectral properties of the phonon resonances in infrared spectra.

We also apply our approach to the Raman case and we show that, due to the different dependence on the high-energy particle-hole transitions, Raman spectroscopy behaves in a qualitative different way with respect to the IR optical probes, explaining the absence of Fano asymmetry and the weak gate-voltage dependence of the phonon strength in Raman spectra [4].

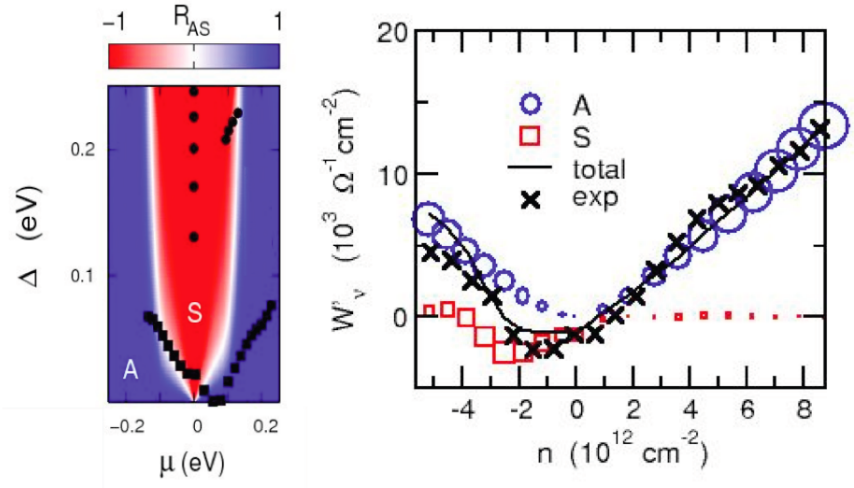

Figure 1: Left panel: phase diagram of phonon mode relevance in the μ vs. Δ space. Blue areas represent the regions where the antisymmetric (A) Eu mode is dominant, red areas where the symmetric (S) mode dominates. Black symbols mark the experimental conditions probed in Ref. [1] (fileld squared) and in Ref. [2] (filled circles). Right panel: different electron-phonon contributions to the total integrated spectral weight $\hat{WO}$ as calculated in the charged-phonon model [3]. The size of the open symbols represents the weight of relative mode. Also shown for comparison the experimental data from Ref. [1].

References

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