Contribution ID: **47** Type: **not specified**

NEMESYS Project- Calibration of the fine-structure constant of graphene by time-dependent density functional theory.

Friday, 15 December 2017 15:40 (20 minutes)

One of the amazing properties of graphene is the ultra-relativistic behavior of its loosely bound electrons, mimicking massless fermions that move with a constant velocity, being inversely proportional to a fine-structure constant αg of the order of unity. The effective interaction between these quasi-particles is, however, better controlled by the coupling parameter α∗g =αg/ε, which accounts for the dynamic screening due to the complex permittivity ε of the many-valence electron system. This concept was introduced in a couple of previous studies [Reed et al., Science 330, 805 (2010), Gan et al., Phys. Rev. B 93, 195150 (2016)], where inelastic x-ray scattering measurements on crystal graphite where converted into an experimentally derived form of α∗g for graphene, over an energy-momentum region on the eV-Å−1 scale. Here, an accurate theoretical framework is provided for α∗g, using time-dependent density functional theory in the random phase approximation, with a cut-off in the interaction between excited electrons in graphene, which translates to an effective inter-layer interaction in graphite. The predictions of the approach are in excellent agreement with the above-mentioned measurements, suggesting a calibration method to substantially improve the experimental derivation of α∗g, which tends to a static limiting value of ~0.14. Thus, the ab initio calibration procedure outlined demonstrates the accuracy of perturbation expansion treatments for the two-dimensional gas of massless Dirac fermions in graphene, in parallel with quantum electrodynamics.

Summary

[Source: A. Sindona, M. Pisarra, C. Vacacela Gomez, P. Riccardi, G. Falcone, and S. Bellucci, Phys. Rev. B 96, 201408(R) –Published 17 November 2017]
Graphene, the two-dimensional (2D) allotrope of carbon with sp2-bonded honeycomb lattice, is the first discovered and currently most studied atomically thin material, due to a variety of potential uses. On the electronic side, the unique properties of graphene stem from its semimetallic band structure around the Fermi energy EF, with the valence (π) and conduction (π∗)energy levels exhibiting a conical dispersion vs the in-plane momentum at the six corners of the (hexagonal) first Brillouin zone (1st BZ), i.e., the Dirac points. This peculiar feature has allowed the development of a quasi-particle description of charge transport, consisting of charge-carriers that behave as massless Dirac fermions on a velocity scale, characterized by the group velocity of the π and π∗ electrons at the Dirac points, i.e., the Fermi velocity vF~c/300, with c~137 being the velocity of light in atomic units. Nonetheless, the quasi-particle interaction in this picture depends on a (bare) effective fine-structure constant αg =1/vF~2.2, being much larger than the vacuum fine-structure constant α=1/c of quantum electrodynamics (QED). Indeed, many-body corrections to vF can significantly lower αg, which, however, contrary to QED, remains too large for perturbation treatments. On the other hand, αg is too small for strong-coupling approaches. Attempts to reduce αg by changing the sup-porting dielectric medium lead to α∗g = αg/ε, where ε is the constant permittivity of the 'background'that embeds the graphene sheet. Even in this case, α∗g remains not far from unity. A more complete 'view'of the interaction strength between the band electrons in graphene amounts to replacing 1/ε in α∗g with the dynamic inverse permittivity, obtained by transferring an energy ω and a momentum q to the system. On these bases, inelastic x-ray scattering experiments were performed [1,2] to determine the many-electron screening in crystal graphite, followed by reconstruction methods to derive the full susceptibility of freestanding graphene, and a diagrammatic formalism structured in powers of α∗g. Here, it is demonstrated that time-dependent (TD) density functional theory (DFT) provides a reliable theoretical framework for the above-mentioned measurements, with a key role being played by the bare Coulomb interaction between excited electrons within the graphene sheet, which reflects in the interlayer interaction in graphite. A substantial improvement on the determination of α∗g is presented, suitable for transfer-red energies from the far-infrared to the extreme ultraviolet, and in-plane momenta up to ~1 Å−1. An exploration on the small in-plane momentum region yields the static limiting value α∗g~0.14, in agreement with [1], which supports the idea that the massless Dirac fermions of graphene experience a suf-

ficiently weak interaction. More importantly, a procedure to extrapolate the effective fine-structure constant of Dirac-cone materials is outlined.

[1] Reed et al., Science 330, 805 (2010)
[2] Gan et al., Phys. Rev. B 93, 195150 (2016)

Primary author: SINDONA, Antonio (CS)

Co-author: BELLUCCI, Stefano (LNF)

Presenter: SINDONA, Antonio (CS)

Session Classification: Session 11