NANO COLLOQUIA 2024 - S3 SEMINAR

Efficient full frequency GW calculations: semiconductors, metals, and... graphene

Thursday May 09, 2024 – 14:30

ON-SITE - S3 Seminar Room, Third Floor, Physics Building
ONLINE - https://tinyurl.com/NanoColloquia

Speaker: Claudia Cardoso - Cnr Nano S3

Abstract

Many-body perturbation theory methods, such as the GW approximation, are the state of the art for the calculation of quasiparticle (QP) properties of a large range of materials. However, evaluating the GW self-energy is often computationally challenging due to the frequency and momentum convolutions. These difficulties were recently addressed by the developments of the multipole approximation (MPA) [1,2] and the W-av [3,4] methods. MPA leads to an accuracy comparable with full-frequency methods at much lower computational cost. W-av drastically improves the convergence of the QP corrections of 2D semiconductors with respect to the Brillouin zone sampling. Here, we present these two theoretical schemes and show examples of the accuracy and computational gains when applied to several prototype systems. We will show that the computational efficiency of MPA and W-av allows us to explore the logarithmic renormalization of the Dirac cone of graphene.

[1] D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, E. Molinari, and A. Ferretti. "Frequency dependence in GW made simple using a multi-pole approximation". Phys. Rev. B 104, 115157 (2021).
[2] D. A. Leon, A. Ferretti, D. Varsano, E. Molinari, and C. Cardoso. "Efficient full frequency GW for metals using a multipole approach for the dielectric screening". Phys. Rev. B 107, 155130 (2023).
[3] A. Guandalini, P. D'Amico, A. Ferretti and D. Varsano. "Efficient GW calculations in two-dimensional materials through a stochastic integration of the screened potential. npj Comp. Mat. 9, 44 (2023).
[4] A. Guandalini, D. A. Leon, P. D'Amico, C. Cardoso, A. Ferretti, and D. Varsano. "Efficient GW calculations via the interpolation of the screened interaction in momentum and frequency space: The case of graphene". Phys. Rev. B 109, 075120 (2024).

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