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Particle-In-Cell Simulations of Quantum Plasmas

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Room-temperature metals and semi-metals, characterized by bound electron gases in near-continuum band structures, can be viewed as cold quantum plasmas. This perspective enables the adaptation of Particle-in-Cell (PIC) simulations, traditionally used for classical plasmas, to model dynamic phenomena in nanophotonics and plasmonics. In our work, we have extended the capabilities of the SMILEI PIC code by implementing four innovative physics modules: (I) initialization of Fermi-Dirac distributed charge species, (II) material boundary conditions tailored for condensed matter interactions, (III) a bound-particle model enabling the simulation of linear dispersive media, and (IV) a framework for modeling massless Dirac fermions to simulate graphene-like materials. These additions provide a versatile and self-consistent platform for exploring dynamic electromagnetic responses in nanophotonic and plasmonic systems [1][2][3].
This talk outlines the integration of these modules into the SMILEI framework and their role in enhancing quantum plasma modeling. We discuss practical considerations during implementation, including adapting the modified Boris scheme for new particle dynamics: bound electrons and massless Dirac electrons, and present benchmark simulations validating the updates. These results highlight the augmented SMILEI code's potential for studying time-dependent phenomena in quantum plasmas, such as interband plasmon resonances and nonlinear Dirac electron dynamics. By sharing these developments, we aim to support further exploration of quantum materials and nanophotonic systems using mesoscopic particle simulations [4].

[1] Ding, W. J. et al. Particle simulation of plasmons. Nanophotonics 9, 3303–3313 (2020)
[2] Do, H. T. B. et al. Electron dynamics in plasmons.
Nanoscale 13, 2801–2810 (2021).
[3] Do, H. T. B. et al. Nonlinear Terahertz Resonances from Ballistic Electron Funnelling. Preprint at https://doi.org/10.48550/arXiv.2411.09
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