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Terahertz Response of Monolayer Graphene:Velocity Gauge Vs Length Gauge

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Graphene, as a zero-bandgap two-dimensional semiconductor with a linear electron band dispersion near the Dirac points has potential to exhibit very interesting nonlinear optical properties [1]. In particular, third harmonic generation of terahertz (THz) radiation should occur both due to the nonlinear relationship between the crystal momentum and the current density, and due to the interaction between interband and intraband parts of the current densities due to the vanishing bandgap [2]. In this work, we investigate two different ways of calculating the nonlinear response of graphene to THz radiation.

There are two different gauges that are commonly employed to study the interaction of electrons in a semiconductor with a THz or optical field: the velocity gauge and the length gauge [3,4] In the length gauge, the interaction of the electrons with the field is given by $\vec{r} \cdot \vec{E}(t)$, while in the length gauge, it is given by $\vec{p} \cdot \vec{A}(t)$. In this work, we derive the nonlinear density matrix equations and current density expressions in the two gauges for graphene in a two band model. We show that if one uses the mass sum rule for the bands, the two methods yield very similar linear conductivities. However, we find that the nonlinear response can be quite different for the two approaches, due in large part to the divergences that arise at zero frequency in the velocity gauge when one uses a basis with a finite number of bands. We conclude that one should use the the length gauge for graphene when calculating the nonlinear THz response.

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