O.33 Electron-phonon beyond Fröhlich: dynamical quadrupoles in polar and covalent solids

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First-principles computations of electron-phonon related properties in polar and covalent solids have gained popularity in the last five years. In polar semiconductors, the long-range electrostatic interactions lead to the dipolar Fröhlich divergence of the electron-phonon coupling matrix elements. This contribution was recently generalized to anisotropic materials, opening up a first avenue for computations of electron-phonon effects in polar materials [1].

In this talk, we include the treatment of quadrupolar fields beyond the Fröhlich interaction in the electron-phonon vertex in semiconductors. Such quadrupolar fields induce additional long-range interactions that have to be taken into account for accurate physical results. We apply our formalism to Si (nonpolar), GaAs, and GaP (polar) and demonstrate that phonon-limited electron mobilities show large errors if dynamical quadrupoles are not properly treated.

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