Nonequilibrium Terahertz Conductivity in Systems with Localized Electronic States

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A broad range of disordered materials contain electronic states that are spatially well localized. These include amorphous inorganic semiconductors, inorganic crystals doped with randomly positioned impurities and organic semiconductors based on conjugated polymers or small molecules. Usual approaches to simulation of ac conductivity rely on Kubo′s formula which expresses the ac conductivity in terms of the mean square displacement of a diffusing carrier. Such approaches therefore assume that carriers are in equilibrium and that they are only slightly perturbed by external alternating electric field. However, in many realistic situations, the carriers are not in equilibrium; a typical example concerns the carriers created by external optical excitation across the band gap of a semiconductor.

In this work we obtain the expression for the optical conductivity in a material with localized electronic states and weak electron-phonon or electron-impurity interaction [1]. The expression is valid for any nonequilibirum state of the electronic subsystem prior to the action of electric field. Particularly, in the case of incoherent nonequilibrium state of the electronic subsystem, the optical conductivity is entirely expressed in terms of the positions of electronic states, their nonequilibrium populations, and Fermi′s golden rule transition probabilities between the states. The same mathematical form of the expression is valid both in the case of electron-phonon and electron-impurity interaction. Moreover, our result for the nonequilibrium optical conductivity has the same form as the expressions previously obtained for the case of equilibrium. The derivation was performed by expanding the general expression for ac conductivity in powers of small electron-phonon or electron-impurity interaction parameter. Our results are expected to be valid at sufficiently high frequencies, such that the period of the electric field is much smaller than the carrier relaxation time. We apply the derived expressions to two model systems, a simple one-dimensional Gaussian disorder model and the model of a realistic three-dimensional organic polymer material obtained using previously developed multiscale methodology [2]. We note that the simple one-dimensional model captures the essential features of the mobility spectrum of a more realistic system. Furthermore, our simulations of the polymer material yield the same order of magnitude of the terahertz mobility as previously reported in experiments.

References

[1] V. Janković and N. Vukmirović, Phys. Rev. B **90**, 224201 (2014).
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