Computation of light absorption in disordered semiconductor alloys based on the localization landscape and the Wigner-Weyl approach

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Light absorption and emission measurements are commonly used to study the electronic and optoelectronic properties of semiconductor alloys, and to characterize devices made of heterostructures of such alloys such as LEDs. These measurements are particularly sensitive to the band edge structure. For example, the absorption frequency threshold is in general affected by several processes: thermal processes, electric fields [1], the electron-hole Coulomb interaction [2], and alloy disorder [3] and the joint effect of the two latter [4]. Alloy disorder corresponds to the random configuration of atoms of different species on the crystal lattice, and consequently, breaks the periodic symmetry of the ion lattice potential. The common tools of solid states physics based on the Bloch theorem must then be adapted.

In order to understand and predict the effect of alloy disorder on the optoelectronic properties of alloys and devices, we present a model of light absorption based on a formulation in phase space for the electronic states and on results from the localization landscape framework [5, 6].

The derived model is simple, computationally efficient and yields good approximations for practical purposes. The simulated absorption coefficient is compared with eigenstates based computations in 1D and 2D, and is shown to be accurate for disorder parameters relevant for InGaN alloys. The absorption model is then applied in 3D for InGaN alloys of different compositions. The impact of the indium concentration on the Urbach tail and on the spatial distribution of the absorbed power are discussed.

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[1] J. D. Dow and D. Redfield, Phys. Rev. B **5**, 594 (1972).
[2] R. J. Elliott, Phys. Rev. **108**, 1384 (1957).
[3] M. Piccardo, C.-K. Li, Y.-R. Wu, J. S. Speck, B. Bonef, R. M. Farrell, M. Filoche, L. Martinelli, J. Peretti, and C. Weisbuch, Phys. Rev. B **95**, 144205 (2017).
[4] A. David, N. G. Young, and M. D. Craven, Phys. Rev. Applied **12**, 044059 (2019).
[5] M. Filoche and S. Mayboroda, Proceedings of the National Academy of Sciences **109**, 14761 (2012).
[6] D. N. Arnold, G. David, D. Jerison, S. Mayboroda, and M. Filoche, Phys. Rev. Lett. **116**, 056602 (2016).