Prediction of Wave Functions Transport Regime Using Machine Learning

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Master thesis in Physics

Electromagnetic waves in correlated disordered structures shows interesting and rich transport properties. Indeed, different light transport regime emerge depending on the degree of correlation and the frequency, but keeping the properties of the scatterers constant. More precisely, at least 5 different transport regimes have been recognized in 2D stealthy hyperuniform structures (SHU) [1]. These 5 different transport regimes are namely transparency [2], diffusion, Anderson localization, pseudo-tunneling [3] and tunneling through complete stop bands [4].
To determine the transport regime associated to a wave function, the method which is usually used is to compute the inverse participation ratio (IPR) [5]. This indicator gives an information on the localization of a wave function and on how many scatterers are covered by the wave function. However, the IPR and its generalized version is not the right tool to determine the transport regime because it cannot account for the 5 different transport regimes.
After the successful use of machine learning techniques in this field [6] and since the IPR does not work, a machine learning approach is tested. For this, a convolutional neural network, EfficientNet [7] is trained with more than 200'000 images of wave functions labeled with their transport regime. After showing that the accuracy of EfficientNet on these wave functions can be bigger than 93%, the generalization capabilities of the network are disussed, as well as its limitations.

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