# The Pauli principle in the Monte Carlo method for charge transport in graphene

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The Monte Carlo method has become a standard tool for the study of transport problems in electronic devices [1], together with the semiclassical ensemble Monte Carlo method (EMC). When the Pauli principle is no longer negligible, however, the EMC suffers from some drawbacks regarding the correct reconstruction of the carrier distribution. Many attempts were made over the years to overcome this problem until a new Monte Carlo scheme which takes into account the Pauli principle correctly was developed (see [3] and references therein). Almost all of these works were based on some convenient approximations in the description of the distribution function or of the scattering terms, with no attention on the free-flight step. Earlier on [4], a novel procedure was developed for silicon, which added the Pauli principle also at the end of the free flight, and which could be used when the degeneracy effects are predominant. Here, we address the question of the correctness of representing the free flight in a quantum perspective, with the application of the Pauli principle, or if it is more appropriate to represent it in a semiclassical way with the Liouville operator. We carry out this study by performing a numerical comparison of the various approaches by looking at the effects on the electron distribution function and on the mean values of energy and velocity in the case of a suspended monolayer graphene. This problem is fundamental in the study of new materials, as graphene, where degeneracy effects are important.

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