Monte Carlo Simulations for 2D Materials: Parallelization Strategy and Degeneracy in MoS_2

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Two-dimensional (2D) materials have stood out in the last years in the search for going beyond Silicon in electronic device applications. Graphene is the best example in this area, although 2D transition metal dichalcogenides are also very well positioned. There is a real need of fully examine the electronic transport in these novel materials using advanced physically based numerical models. Among them, ensemble Monte Carlo (MC) simulations offer great advantages due to their intrinsic relation to the nanoscale stochastic and quantum-mechanical transport processes.
Our in-house ensemble MC simulator has been successfully employed in the study of graphene, silicene or transition metal dichalcogenides as molybdenum disulfide (MoS_2) [1, 2, 3]. In the present work, for the first time, we have focused on the analysis of the effects of degeneracy in MoS_2 using a MC tool taking into account Pauli exclusion principle and the renormalization of the electron-phonon coupling through the addition of the dielectric function [4, 5, 6, 7].
On the other hand, in order to expand the possibilities of our MC simulator and to lighten the large computational burden linked to these simulations, we have also developed a parallelization strategy of our code. The MC method for electron transport in semiconductors is based on several numerical and computational algorithms used to approximate complex mathematical expressions (related to the probabilities of scattering in solids, etc.) using repeated random sampling, even if they are deterministic [8]. The parallelization is not a trivial task due to the fact that the motion of the set of particles, mimicking Boltzmann Transport Equation (with classical free flights interrupted by quantum-mechanical scatterings) depends on their prior motion and cannot be performed independently [9]. Besides, the parallelization of the developed sequential simulator makes the transition to a parallel MC simulator even more challenging.
The Message Passage Interface (MPI) is used to parallelize our MC simulator (written in Fortran programming language). In the first instance, the implemented physical model and the features of the simulator are needed to be analysed in depth.
Results for the impact of degeneracy in MoS_2 and the improvement of the CPU times in the simulation of 2D materials will be discussed.

References

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Acknowledgments
This work has been funded by research project TEC2016-80839-P financed by Ministerio de Economía y Competitividad (Spain) and FEDER (European Union), JCYL (Regional government) and European Socia Fund via PhD Grant SA176-15, and the Project HPC-EUROPA3 (INFRAIA-2016-1-730897), with the support of the EC Research Innovation Action under the H2020 Programme.