Simulation of hopping conductivity in electron glasses with the parallel rejection algorithm

Matteo Palassini[1], Ezequiel E. Ferrero[2], and Alejandro B. Kolton[3]
[1]Departament de Física de la Materia Condensada, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain
[2]Université Grenoble Alpes, LIPHY, F-38000 Grenoble, France and CNRS, LIPHY, F-38000 Grenoble, France
[3]CONICET, Centro Atómico Bariloche, 8400 Bariloche, Argentina

A common limitation of Markov-chain Monte Carlo (MC) methods is low acceptance. In equilibrium MC this problem can sometimes be circumvented with a clever choice of the MC moves, which can be chosen with a certain freedom as long as the Markov chain converges to the probability distribution of interest. Such freedom is not allowed in kinetic Monte Carlo (KMC), in which the MC moves are dictated by the physical dynamics to be simulated.

We recently introduced a general "parallel rejection" (PR) algorithm to address the problem of low acceptance, which is especially suitable for implementation on Graphics Processing Units (GPUs), easily available and inexpensive platforms for massively parallel computing [1].

We apply PR to the KMC simulation of the hopping conduction in disordered systems of localized electrons with long-range interaction, known as electron glasses or Coulomb glasses [3]. Simulations of these systems are plagued by the slow equilibration typical of frustrated systems, complicated by the long-range interaction and by the need to simulate very low temperature to access the variable-range hopping regime. They are thus plagued by very low acceptance.

For this particular application, PR can be seen as a parallelization of the "mixed" algorithm of Refs. [2], which can be further accelerated in GPUs by efficiently parallelizing the N local energy updates that, due to the long-range interaction, are required after each elementary MC move in a system with N sites.

We present here results in three dimensions which show that the parallel rejection algorithm outpaces the serial implementation of the mixed algorithm by several order of magnitude, thus allowing us to compute the conductivity down to very low temperatures. In particular, we provide evidence of a scaling relation for the relaxation of the conductivity at different temperatures.

[1] E. E. Ferrero, A. B. Kolton, and M. Palassini, AIP Conference Proceedings **12**, 71 (2014).

[2] D. N. Tsigankov, E. Pazy, B. D. Laikhtman, and A. L. Efros, Phys. Rev. B **68**, 184205 (2003)

[3] M. Palassini, *Electron Glasses*, Contrib. Sci. **11**(2), 163 (2015).
(revistes.iec.cat/index.php/CtS/article/viewArticle/142168)