Particle-grid techniques for semiclassical and quantum transport simulations

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Particle simulation techniques utilizing classical or quantum weights commonly involve a phase space grid for calculation of averages. Properties of alternative particle-grid simulation strategies are investigated by using an experiment highly sensitive to variance. It is provided by the fine structure of entangled electron states subject to scattering with phonons. As the process of evolution describes decoherence and transition from quantum to classical our analysis concerns both transport regimes. An algorithm based on randomization-annihilation (RA) of particles shows better performance than an Ensemble Monte Carlo (EMC) method.

Efforts for a generalization towards quantum transport exist since more than two decades [1] and gave rise to Monte Carlo techniques which rely on the numerical aspects of the transport description [2]. Quantum particles have recently been shown as a viable approach for the simulation of nanostructures, which bridge the gap between purely coherent and semi-classical transport regimes [4]. Common features for such particles are that they evolve along classical trajectories, while the quantum information is carried by a dimensionless quantity – affinity or sign, which may be associated with the semi-classical particle weights. The total weight – quantum or semi-classical – accumulated around a given phase space point along with the local value of a generic physical quantity are used for evaluation of its averaged value. A phase space grid is commonly utilized to store the weight of all particles at consecutive time steps. Usually the same particles continue the evolution. Alternatively the weight can be redistributed between novel particles [3], which survive only within a single time step. The peculiarities of these approaches are explored with the help of several notions similar to cellular automata simulations [6].

Previously investigated algorithms make use of individual numerical particles, keeping track of each of their positions and weights, for their operation. The quantum nature of the problem under investigation is expressed by the existence of positive as well as negative weights. We now present an algorithm which moves towards indistinguishable particles.

The phase space associated with the simulation domain is subdivided into cells which are used to store the number of particles in the cell as well as the total weight associated with the sum of all particles. Initially, the cells are seeded with values corresponding to the initial condition of a coherent state composed of two Gaussian wave packets [5]. A cell with non vanishing content is then assigned a number of particles. Particles are then generated from a given cell each carrying an equal piece of the stored total weight, until the cell is emptied such that the particles originating from a cell are not distinguishable by their weights. The exact starting point is chosen at random from within the cell.

The particles then evolve for a given time step after which the weight is accumulated in a cell corresponding to the final position. At the same time the counter of particles in the cell is increased. This on the one hand ensures the conservation of the number of particles, while on the other hand implements an annihilation scheme for particles of opposing weights.

The excellent agreement of the EMC and RAMC, which has superior numerical behaviour, is shown in the figures. The introduced algorithm thus not only has the benefit of a reduced memory footprint as not the entire ensemble of particles needs to be kept in memory, but also results in a lower statistical error.

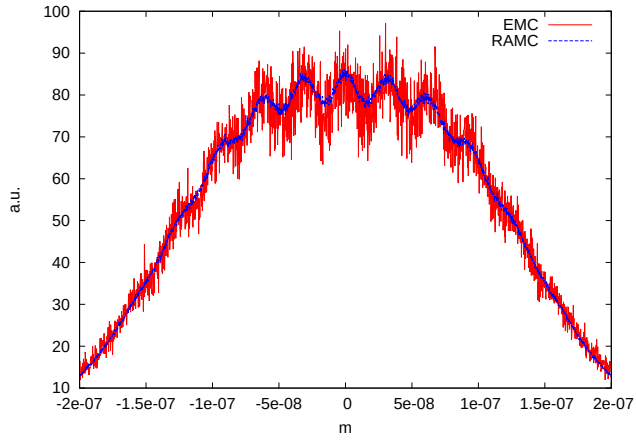

Fig. 1. Evolution of the density of a state comprised of two entangled Gaussians after 400fs. The EMC and the RAMC algorithms show excellent agreement, with the latter demonstrating numerical superiority.

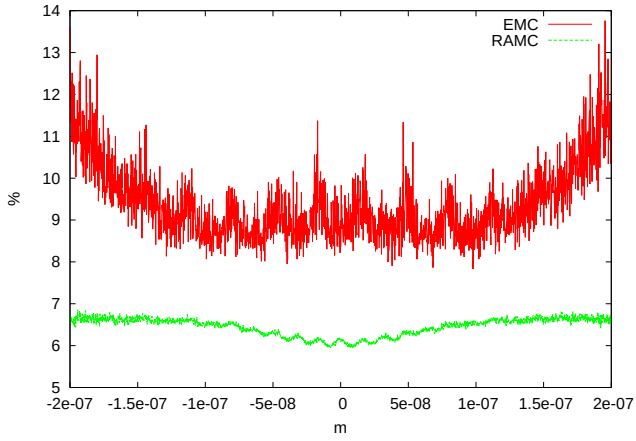

Fig. 2. The RAMC algorithm produces lower relative errors than the EMC algorithm in the case of densities.

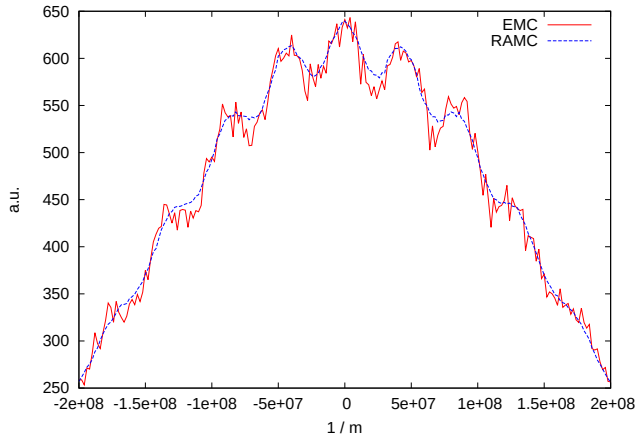

Fig. 3. Evolution of the momentum distribution of a state comprised of two entangled Gaussians after 400fs. The EMC and the RAMC algorithms show excellent agreement, with the latter demonstrating numerical superiority.

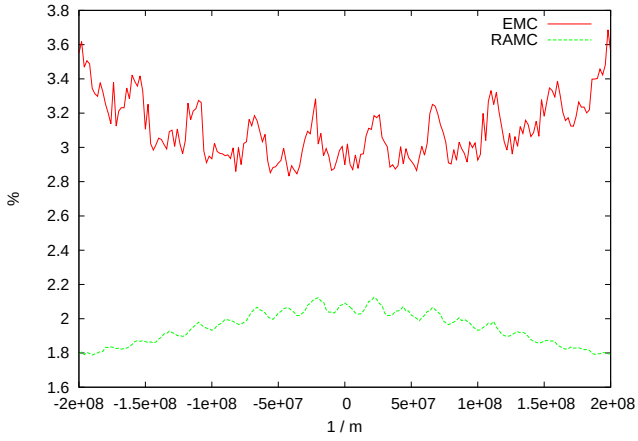

Fig. 4. The RAMC algorithm produces lower relative errors than the EMC algorithm for the momentum distribution.

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