Particle-Grid Techniques for Semiclassical and Quantum Transport Simulations

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***Abstract*— Particle simulation techniques utilizing classical or quantum weights commonly involve a phase space grid for the 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 of particles shows better performance than an Ensemble Monte Carlo method.**

Introduction

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 nano structures, 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, e.g., 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 newly generated particles [3], which survive only for a single time step. The peculiarities of these approaches are explored with the help of several notions similar to simulations using cellular automata [6].

The Randomization-Annihilation Monte Carlo (RAMC) Algorithm

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 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].

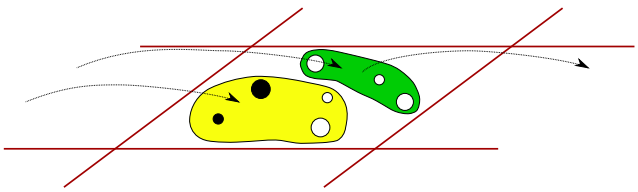

Fig. 1. Particles (black – positive, white – negative) are recorded as they enter the cell. Opposing weights are annihilated (yellow). The surviving weight (green) is emitted as particles from the cell by randomizing the starting position from within the cell. The number of emitted particles is the same as the number of entering particles.

Figure 1 illustrates the operation of the RAMC algorithm. Each of the cells keeps track of the particles entering. Not only are the weights recorded, but also the number of particles. The number of

particles is maintained, whereas opposing weights (illustrated in black and white) are canceled (particles marked in yellow). The surviving weight (particles marked in green) is then emitted divided equally among the number of total particles which have entered the cell.

Particles are then generated from a given cell each carrying an equal piece of the stored total weight, until the cell is emptied. The particles originating from a cell are not distinguishable, e.g., by their weights. The exact point of origin is chosen at random from within the cell.

The particles then evolve for a given time step using Newton's trajectories after which the weight is accumulated in the 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 aggregating and randomizing nature of the RAMC algorithm also has the added benefit of reducing the amount of memory required at run time, since not each and every particle must be tracked individually during the whole duration of the simulation.

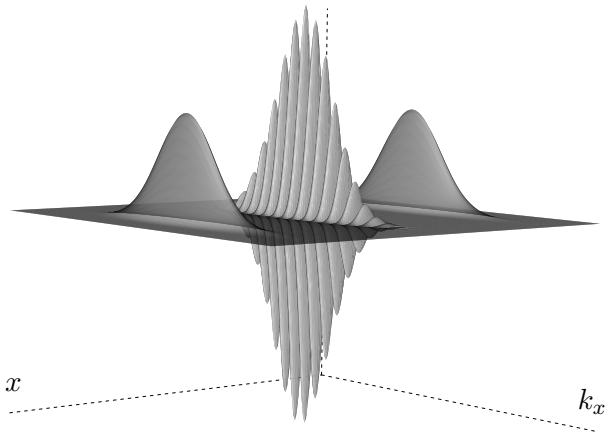

Fig. 2. Initial quantum state used to gauge the EMC and RAMC algorithms.

Application & Results

The system the EMC and RAMC algorithms are applied to begins in a purely quantum state, due to two entangled Gaussian wave packets. It is described by the expression

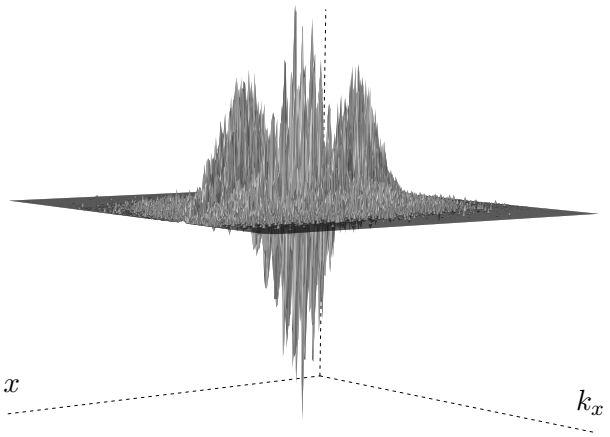

Fig. 3. Scattering processes redistribute the initial distribution progressively annihilating the quantum information.

$$f_w^0(x,k_x) = e^{-k_x^2\sigma^2}\left(e^{-\frac{(x-a)^2}{\sigma^2}} + e^{-\frac{(x+a)^2}{\sigma^2}} + e^{-\frac{x^2}{\sigma^2}} cos\,(k_x 2a)\right)$$

The initial state is constructed such as to incorporate a well pronounced oscillatory term, which may be interpreted as formed by particles with positive and negative weights. Figure 2 depicts this initial configuration including the strong oscillations.

From the quantum setup it then evolves towards a classical configuration. The fine quantum characteristics are suppressed as the system evolves and correlations are destroyed due to the non-coherent scattering processes, which redistribute the phase space distribution. Figure 3 shows the the effect of the redistribution due to scattering, the initially fine structure in the central part is especially susceptible to this process. This makes the evolution sensitive to the variance of the employed algorithm. A possible reduction provided by the RAMC algorithm is therefore of great interest in this particular case.

Figure 4 compares the densities computed using EMC as well as the RAMC algorithms after $400fs$ of evolution. While the quantum features are still observable in both, the lower variance algorithm makes them much more apparent. Figure 5 shows the estimates for the relative errors computed for the densities for each of the algorithms.

Figure 6 shows the distribution of momenta after $400fs$ of evolution. The observation of reduced variance is further reinforced by comparing the relative errors, which are provided in Figure 7.

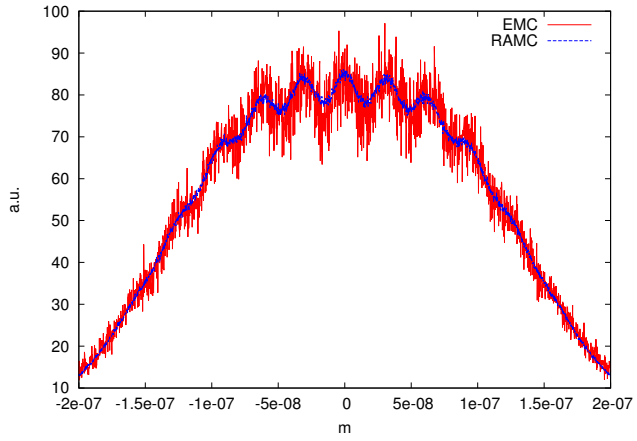

Fig. 4. Evolution of the density of a state comprised of two entangled Gaussians after 400fs. The EMC and the RAMC algorithms show excellent agreement, with the latter demonstrating numerical superiority.

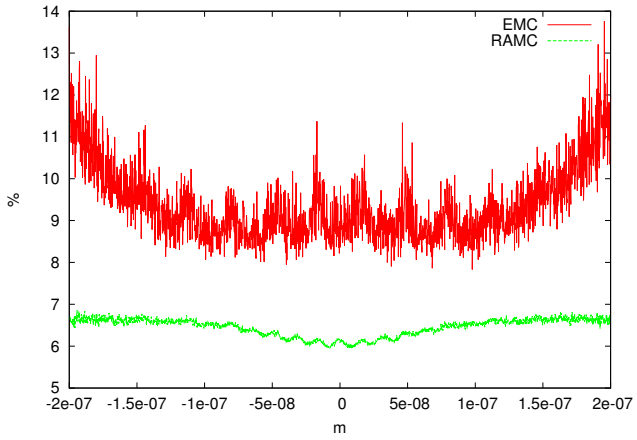

Fig. 5. The RAMC algorithm produces lower relative errors than the EMC algorithm in the case of densities.

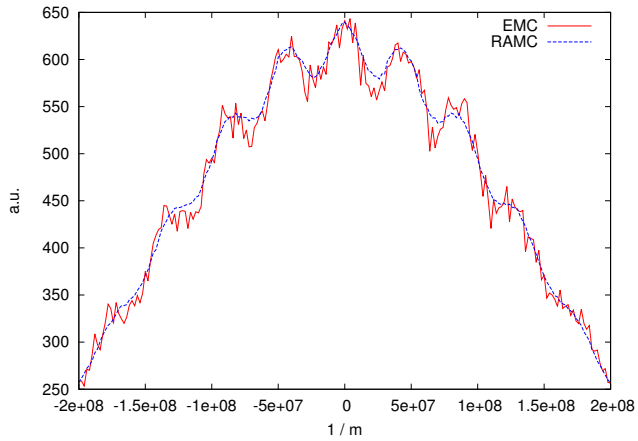

Fig. 6. Evolution of the momentum distribution of a state comprised of two entangled Gaussians after 400fs. The EMC and the RAMC algorithms show excellent agreement, with the latter demonstrating numerical superiority.

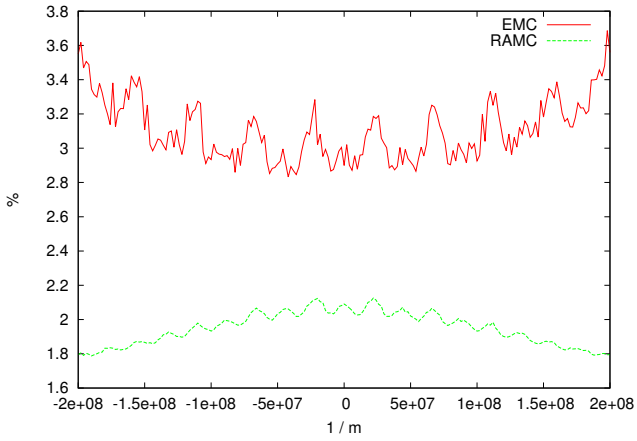

Fig. 7. The RAMC algorithm produces lower relative errors than the EMC algorithm for the momentum distribution.

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

ACKNOWLEDGMENT

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