The Ultimate Equivalence Between Coherent Quantum and Classical Regimes

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The difference between the classical and the quantum mean values of a physical quantity associated with the evolution of an initial state may be evaluated by an estimate [1], which vanishes for up to quadratic potentials. In this case the commutator coincides with the Poisson bracket and the physical aspects are determined by the initial condition only. This ultimate parity may be used to setup benchmark experiments testing the properties of computational approaches. In particular, in the Wigner picture it holds:

$$\int dk' V_w(k-k')f(x,k',t) = -\frac{eE\partial f(x,k,t)}{\hbar\partial k} \qquad (1)$$

showing the equivalence of the ballistic Boltzmann and coherent Wigner evolution for linear potentials $V(x) = Ex$. The choice of an initial condition $f(x,k,0) = N\delta(k)\delta(x)$ discards all quantum effects, so that the evolution is a simple acceleration of classical particles over a Newton trajectory. Why has this duality not yet been used as a reference for validation of Wigner transport simulation methods? The reason is that according to (1) V_w is a generalized function: $V_w(k) = \frac{eE}{\hbar}\delta'(k)$, which precludes any exact numerical treatment: even the standard, infinitely coherent in space, definition of the Wigner potential [2] diverges. This research aims at both, the development of an asymptotic approach as well as a validation of our Wigner particle model for this extreme case. The model accounts for mixed initial and boundary conditions and entangles particle attributes such as drift, generation and sign of the ergodic counterpart [3] with the concepts for momentum quantization, indistinguishable particles and annihilation at consecutive time steps. The key parameter in this approach is the finite coherence length L giving rise to the quantization $\Delta k = \pi/L$ of the momentum subspace, and a discrete Fourier expansion

$$V_w(n) = \int_{-L/2}^{L/2} \frac{e^{-in\Delta ks}}{i\hbar L}\Delta V(x\pm s)ds = -\frac{eEL}{\hbar\pi n}cos(\pi n)$$

The quantization imposes rules of cellular automata on the Boltzmann evolution [4]: The probability for a transition during a time dt to the next node n in field direction is proportional to the acceleration $dk = eEdt/\hbar$. This leads to a reference process, where the number of particles placed at the initial node gradually decreases in favour of the corresponding increase on the next node. Newton's law is recovered in the limit $L \to \infty$. The challenge now is to emulate the same process by generation of signed particles according to $V_w(n)$, which reside at a momentum grid during the evolution and may annihilate if having: opposite sign; identical phase space coordinates; identical evolution times. This illustrates their indistinguishability. Our simulations indeed demonstrate this behaviour: Figure 1 shows the initial peak which drops so that at $0.53ps$ the two adjacent nodes contain an equal number of particles, while after $1ps$ the transition is complete. However, an additional phenomenon is revealed by this evolution process: a pattern of oscillating values appears. We associate this with the fact that the equivalence between quantum and classical evolution is asymptotic only. The discrete quantum system is disturbed by the violation of the uncertainty principle in the initial condition. Indeed, with an increase of L the magnitude of the oscillations decreases, Figure 2. Another interesting phenomenon is the pulsing of the pattern in time: during a transition the oscillations are much higher than at its end, as if the solution tends to the classical shape at discrete points in time, Figure 1 and Figure 3. For $E = 10^4 V/m$ and $L = 200nm$ these instants are consistent with Newton's law: $\Delta k = eE\Delta t/\hbar$. It also validates the robust behaviour of our technique: the $5ps$ solution is obtained without any distortion due to annihilation. Figure 4 shows the dramatic increase of computational effort with increasing evolution time and the importance of annihilation to keep particle numbers under control. The fine structure and asymptotic behaviour of the analysed quantum process makes it an ideal candidate for benchmark simulations.

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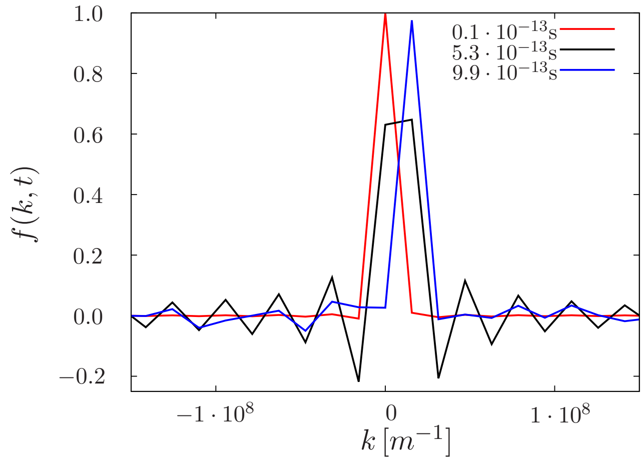

Fig. 1. The effect of the accelerating force is replaced by the Wigner potential with generation of positive and negative particles which reside on the grid in momentum space. The decrease of the initial peak is entirely due to the generation of negative particles at the zero node. These annihilate with the positive counterparts leading to a decrease of the initial condition. On the next node to the right positive particles are generated. The net effect is as in the cellular automata reference process. The transition of the peak between two neighbouring nodes is accompanied by increased oscillations, which are subside once the transition is complete.

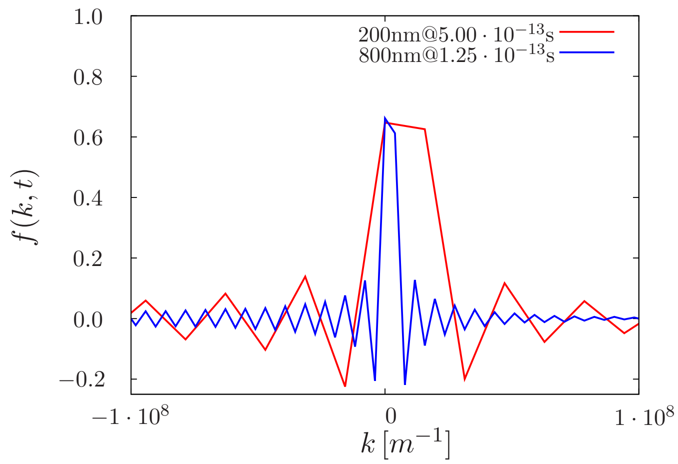

Fig. 2. An increase of the coherence length reduces the magnitude of the oscillations, demonstrating the expected asymptotic behaviour. The corresponding decrease of Δk reflects on the time required for half transfer, according to Newton's law, by reducing it 4 times.

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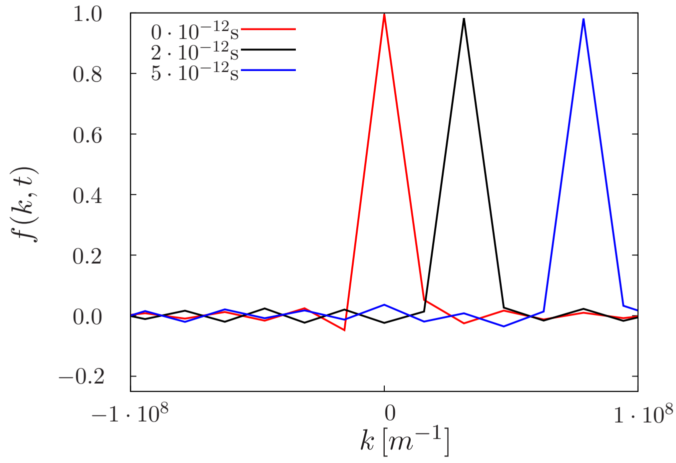

Fig. 3. The initial peak moves robustly for 5ps demonstrating the lack of any distortion due to the annihilation of particles. Points in time corresponding to Newton's law have much lower oscillations.

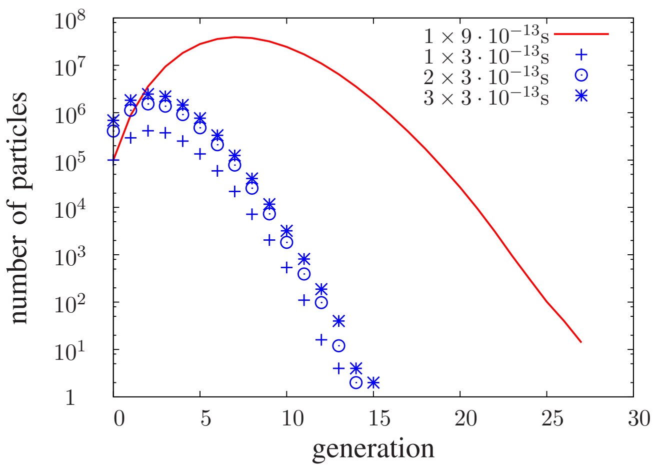

Fig. 4. An increase of the time step dramatically increases the number of generated particles as can be seen by comparing the number of generated particles for $9 \cdot 10^{-13}$s with $3 \times 3 \cdot 10^{-13}$s.

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