Stochastic Formulation of Newton's Acceleration

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Abstract. The theoretical equivalence of the Wigner and ballistic Boltzmann equations for up to quadratic electric potentials provides the convenient opportunity to evaluate stochastic algorithms for the solution of the former equation with the analytic solutions of the latter equation - Liouville trajectories corresponding to acceleration due to a constant electric field. The direct application of this idea is impeded by the fact that the analytic transformation of the first equation into the second involves generalized functions. In particular, the Wigner potential acts as a derivative of the delta function which gives rise to a Newtonian accelerating force. The second problem is related to the discrete nature of the Wigner momentum space. These peculiarities incorporate unphysical effects in the approximate Wigner solution, which tends to the Boltzmann counterpart in a limiting case only.

Operator mechanics are the established representation of quantum mechanics, where the evolution of expectation values of physical quantities are given by operators $\hat{A}$ along with a commutator bracket and an Hamiltonian operator. This is a departure from the classical descriptions of phase spaces where the Hamiltonian and the Poisson bracket impress the space's geometry on the equations of motion. The Wigner formalism [1] is a return to a phase space description of quantum systems and their evolution. In the case of quantum systems the phase space accommodates features not found in the classical case. Where the Liouville component of the Boltzmann equation is governed by the first derivative of the electric potential - the electric field, quantum evolution is determined by the Wigner integral, which accounts for the entire potential in a nonlocal manner. By performing a Taylor expansion of the Wigner integral it is possible to link derivatives of the potential to powers of $\hbar$. Classical systems then appear by a limit of $\hbar \to 0$, which in this case causes only the linear component, the electric field, to remain. This also means that in the case of a linear potential the Wigner equation reduces to the ballistic Boltzmann equation and the nature, classical or quantum, is determined purely by the initial condition. From the multitude of purely mathematically available solutions only a subset is physically viable. In classical systems this requires all states to be nonnegative, which also allows for a direct interpretation as densities. In the case of a quantum system, on the

other hand, this means that a legitimate quantum state must conform to the uncertainty relation [2, 3].

Since the nature only depends on the initial state, it offers a test facility where simulations for quantum simulations may be examined and tested. The generalized functions required for the treatment of the Wigner transport have made application difficult in direct numerical treatment.

Here, an ensemble particle algorithm for general transport regimes determined by initial and boundary conditions and transients is presented. It uses annihilation of indistinguishable particles at consecutive time steps and is rooted in the use of a quantized momentum space. Force effects are introduced exclusively using the Wigner potential, so that individual particles are unaccelerated as they evolve according to the fieldless Liouville operator of the Wigner equation.

1 Monte Carlo Algorithm

The foundation of the algorithm is the reformulation of the problem as a Fredholm integral equation of the second kind, which can be solved by a Neumann series. The series is evaluated using a Monte Carlo approach. Newton trajectories link the individual terms of the series, where the integral kernel is applied repeatedly. Thus the scheme can be presented as comprised by the two major components

- Evolve along a Newton trajectory
- Apply the kernel as a scattering event
- Record

The Newton trajectories used are exactly the same as in a purely classical set up without force.

A representation of the kernel responsible for the scattering transitions, is needed. We employ a discretized version [4] of the originally continuous Wigner potential. Choosing a finite coherence length L also fixes a finite delta in momentum space proportional $\sim 1/L$. When using wave numbers to represent momentum space, as is customary in the field of solid state physics, this yields $\Delta k = \pi/L$. This discrete approach allows for the identification of momenta with integers. The scattering introduced in this manner deviates greatly from classical transport simulations. Where the kernel in classical transport descriptions is positive definite, this is no longer the case in the quantum setting. This requires the introduction of opposing signs for the particles to accommodate the action of the kernel on a particles. Where in a classical case the kernel will act on any given particle and simply may change its state in a possibly discontinuous manner, the Wigner kernel will spawn a pair of new particles from the initial particle. The interaction with the Wigner potential occurs after traversing the trajectory for a certain time. The interaction can be expressed as:

$$\Gamma(\mathbf{r}, \mathbf{m}, \mathbf{m}') = V_W^+(\mathbf{r}, \mathbf{m} - \mathbf{m}') - V_W^-(\mathbf{r}, \mathbf{m}' - \mathbf{m}) + \gamma(\mathbf{r})\delta_{\mathbf{m},\mathbf{m}'} \tag{1}$$

$\mathbf{m}$ and $\mathbf{m}'$ are integers representing the initial and final nodes in momentum space, respectively. The antisymmetry of the Wigner integral, which acts as the scattering source, enforces

$$V_w^+ = max\big(V_w, 0\big), \qquad V_W^-(\mathbf{m}) = V_W^+(-\mathbf{m}) \tag{2}$$

so that the generation of the two new particles is actually linked. A single choice l remains, which is the offset of the new states from the original momentum node m. When choosing the signs of the generated particles, the sign of V_W must be considered. In case V_W is positive, the particle at the position of the final node $m + l$ retains the sign of the generating particle, while the particle at $m - l$ is constructed with the inverted sign. In case the Wigner potential is negative, the signs of the newly spawned particles are flipped. This process of generation is depicted in Figure 1. The left side shows the case of $V_W > 0$, while the flip of the generated signs is shown in the right part of the figure.

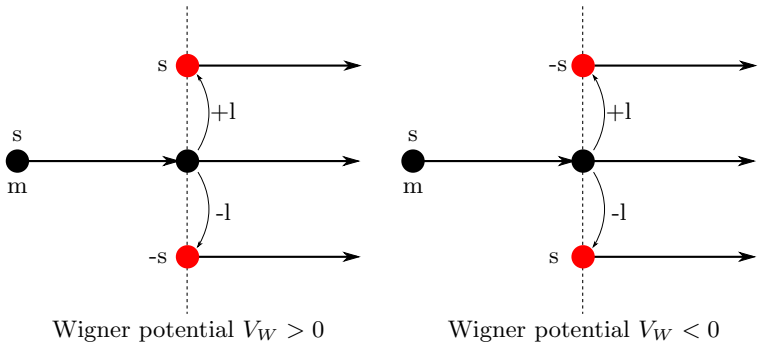

Fig. 1. The signs of the generated particles depend not only on the sign of the original particle, but also on the sign of the Wigner potential at the generating location.

The particles are of opposite signs and each moved in momentum space from the original particle's momentum. In addition to the two newly spawned particles due to interaction with the Wigner potential, the original particle continues along the original trajectory unperturbed, due to the δ function in Equation 1, as is also depicted in Figure 1. Thus, after such an scattering event, instead of the single original particle, now three particles must be processed, each of which not only needs to be processed further but can also generate new particle in the same manner. Thus the total number of particles increases exponentially. This makes it essential to have a means of reducing the number of particles again.

The mechanism counteracting the generation of particles employed in the presented algorithm is annihilation at the time of recording; which marks the end of any chosen time step. Two particles at the same position at the same time but of opposite sign not only have not net contribution to the value of a recording estimator, they also annihilate each other. This means that neither of the two

opposing particles will continue to evolve. Thus the number of overall particles is reduced by two. Since it is necessary for two particles to be at the same place at the same time, the phase space must be subdivided into cells in order to make annihilation feasible, as otherwise the probability of two particles meeting would be zero. The discrete momentum space is already inherently subdivided into a finite set of cells identifiable by the integer indexed nodes. The number of nodes in the momentum component is linked to the resolution selected in space. The number of nodes required to fill the characteristic length L used to obtain V_W is identical to the number of nodes required for momentum quantization.

2 Numerical Analysis

The outlined algorithm for quantum transport is applied to a test configuration consisting of a single peak in the centre of the phase space. It thus is a discrete and finite model of a delta function. From a physical point of view this setting violates the uncertainty relation inherent to quantum phenomena, but since the setting is such that the nature of the system is determined entirely by the condition placed within it, it is expected that this classical initial state should also yield classical results, even as it is subjected to quantum evolution.

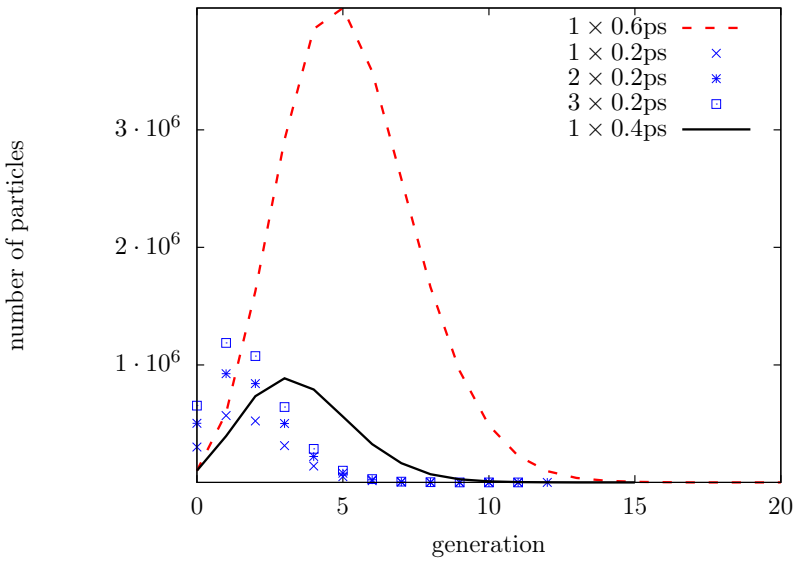

Fig. 2. The length of a time step determines the number of generation before annihilation. When tripling the length of the time step, the shorter time step's number appears almost negligible.

Figure 2 shows how the number of particles depends on the length of the time step and how particles are generated not only from the initial particles.

The initial particles, comprising Generation 0, create an avalanche of subsequent particles. As the time step is increased the number of generated particles and with it the computational burden increases drastically. This can be attributed not only to the fact, that for a fixed probability of interaction with V_W, more particles will be spawned by the primary particles, but also to the circumstance, that the generated particles themselves have a long time span to again generate new particles. The maximum of particles is reached in the 7th generation, after which the number of new particles declines, since the average time remaining until the end of the time step makes generation less probable.

Since the computational burden increases so dramatically when extending the time step, the question arises, if calculations using a series of several shorter time steps will produce results matching a single longer one. As can be seen in Figure 3, the agreement between the different strategies to reach an absolute time is excellent. This indicates that by substituting one long time step by several

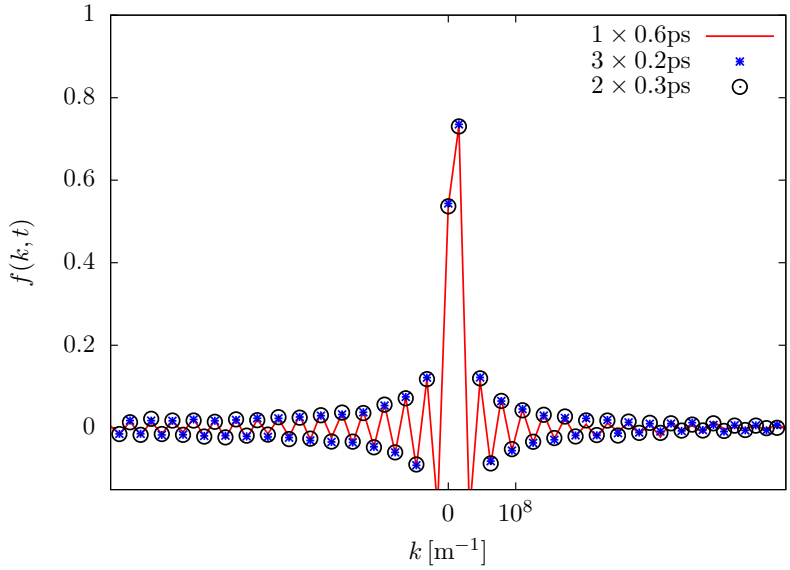

Fig. 3. Choosing a single long time step yields the same results as choosing several shorter time steps, as can be observed for the case of a single 0.6ps time step vs two 0.3ps and three 0.2ps time steps.

shorter ones it is possible to save considerable computational effort, as after each time step the number of particles is reduced by annihilation.

Figure 3 also shows oscillations of the distribution including negative values. This nonphysical behaviour is attributed to the fact that the initial condition used here is in violation of the uncertainty principal required in the quantum setting.

Furthermore, Figure 3 also shows the process of transition from the initially occupied node at 0 to the node at 1. The transition is worth examining in more detail, since it reveals that the transition now occurs as in cellular automata [5].

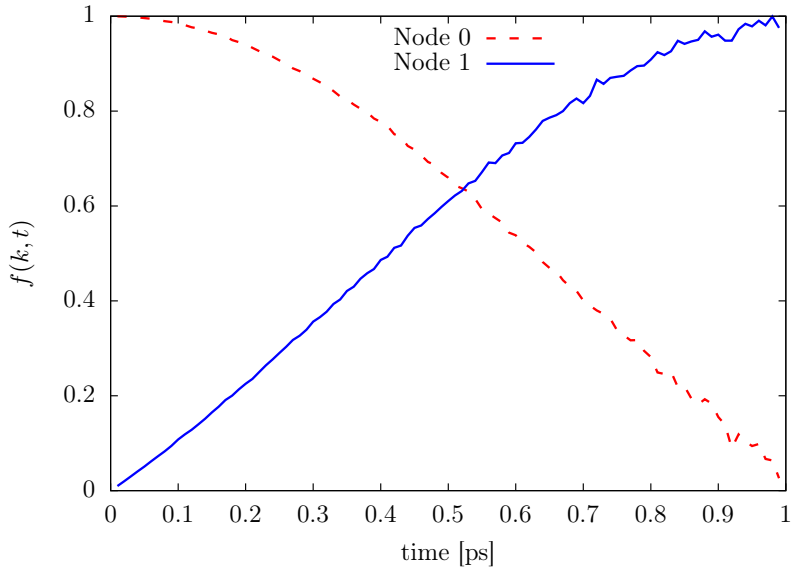

Fig. 4. The densities at the Node 0, which holds the initial condition, and Node 1, which is the first to be occupied. Particles are *not* transferred continuously from node to node until all reach the destination node. Instead the node occupancy is controlled by a generation of positive and negative particles.

Figure 4 resemble a particles transition from one node to another node. The intermediate time regime, where the initial peak has already decreased, while the target has not yet fully formed, is entirely controlled by generation of positive and negative particles and a subsequent annihilation. An analysis of this process will be presented in the sequel. Now we note at Figure 5 the reconstitution of the initial distribution at the target node: the momentum of the particles increases, which corresponds to acceleration but this time without an explicite action of the field. Another interesting physical aspect of the density is the substantial reduction of the spurious oscillations observed in Figure 3. The quantum system is closest to the classical counterpart at dicrete points in time and momentum. At the limit $\Delta k \to 0$ which corresponds to infinite L and thus the continuous case the behaviour becomes classical.

Investigating the manner in which the algorithm moves particles in more detail it is possible to elucidate how the force term is accommodated by purely relying on the mechanism of the Wigner potential V_W. Given a number of particles N_0 located at a given node of a phase space grid a certain number will be

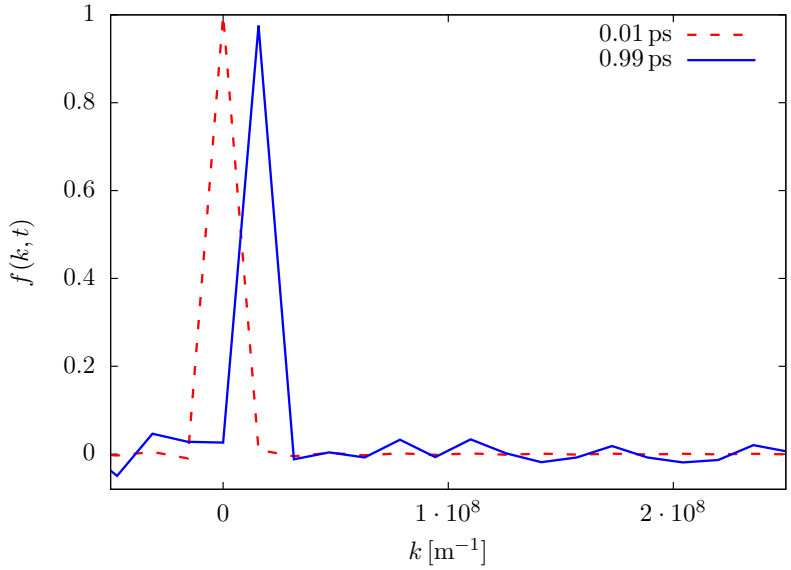

Fig. 5. At times corresponding to Newton's law, the peaks not only reappear but also the nonphysical oscillations are dampened to a minimum.

scattered as they evolve along a Newton trajectory. Even without knowing this number it is possible to examine the ratios of how they will be distributed if we know V_W. In the case under investigation, V_W at the nodes was calculated for a constant electric field to the form of:

$$V_W(n) = \frac{(-1)^{n+1}}{n} \quad \forall n \neq 0, \qquad 0 \quad n = 0 \tag{3}$$

By following the described algorithm the following table is obtained, which shows how many particles are assigned to which node. The common factors are denoted by N_x, where x gives the generation of the particle. The sign of the factor indicates the signs assigned to the particles generated for the particular node.

0	0	0	N_0	0	0	0
$-\frac{1}{3}N_1$	$\frac{1}{2}N_1$	$-N_1$	x	N_1	$-\frac{1}{2}N_1$	$\frac{1}{3}N_1$
$-\frac{1}{2}N_2$	N_2	x	$-N_2$	$\frac{1}{2}N_2$	$-\frac{1}{3}N_2$	$\frac{1}{4}N_2$
$\frac{1}{4}N_2$	$-\frac{1}{3}N_2$	$\frac{1}{2}N_2$	$-N_2$	x	N_2	$-\frac{1}{2}N_2$
$-\frac{1}{2}N_2$	x	$\frac{1}{2}N_2$	$-\frac{1}{2}\frac{1}{2}N_2$	$\frac{1}{3}\frac{1}{2}N_2$	$-\frac{1}{4}\frac{1}{2}N_2$	$\frac{1}{5}\frac{1}{2}N_2$
$-\frac{1}{5}\frac{1}{2}N_2$	$-\frac{1}{4}\frac{1}{2}N_2$	$\frac{1}{3}\frac{1}{2}N_2$	$-\frac{1}{2}\frac{1}{2}N_2$	$\frac{1}{2}N_2$	x	$-\frac{1}{2}N_2$
x	$-\frac{1}{3}N_2$	$\frac{1}{2}\frac{1}{3}N_2$	$-\frac{1}{3}\frac{1}{3}N_2$	$\frac{1}{4}\frac{1}{3}N_2$	$-\frac{1}{5}\frac{1}{3}N_2$	$\frac{1}{6}\frac{1}{3}N_2$
$\frac{1}{6}\frac{1}{3}N_2$	$-\frac{1}{5}\frac{1}{3}N_2$	$\frac{1}{4}\frac{1}{3}N_2$	$-\frac{1}{3}\frac{1}{3}N_2$	$\frac{1}{2}\frac{1}{3}N_2$	$-\frac{1}{3}N_2$	x

The table reveals several peculiarities: The signs of the contribution to the originating node are negative, while they are all positive for the first node to the right. For the remainder of the nodes, the signs are mixed. This supports the conjecture that the algorithm indeed allows to model the effects of force by purely relying on the interaction with V_W. The initial peak is moved by being annihilated by the particles of opposing sign and reconstructed at the neighbouring node.

3 Conclusion

An algorithm for quantum transport has been presented. Its main features include the use of a quantized momentum space and discrete selection rules for the scattering. The discrete nature of the momentum component works very well in conjunction with the employed annihilation scheme, which helps to reduce the number of generated signed particles.

It was shown numerically that it is possible to utilize short time steps to iterate to a longer duration in a stable manner. This is important due to the significant increase of particle generation with the extension of the time step.

Furthermore, an explanation has been provided, how this algorithm accelerates particles without explicitly incorporating a force term.

Finally an interesting mixture of quantum and classical phenomena have been observed in the behavior of the modeled transport process.

Acknowledgements

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