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CAIM
ISSN 2038-0909

Commun. Appl. Ind. Math. 10 (1), 2019, 20–30 DOI: 10.2478/caim-2019-0009

Research Article

Wigner Monte Carlo simulation without discretization error of the tunneling rectangular barrier

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Communicated by Renato Spigler
Received on 10 26, 2018. Accepted on 01 23, 2019.

Abstract

The Wigner transport equation can be solved stochastically by Monte Carlo techniques based on the theory of piecewise deterministic Markov processes. A new stochastic algorithm, without time discretization error, has been implemented and studied in the case of the quantum transport through a rectangular potential barrier.

Keywords: Nanostructures, Wigner transport equation, Direct simulation Monte Carlo
AMS subject classification: 82D80, 82S30, 65M75

1. Introduction

Modelling of electronic transport in nanometer systems requires a theory that describes open, quantum-statistical systems which cannot be provided simply from the Schrödinger equation. Several formulations of quantum transport have been employed practically, such as those based on the density matrix, non-equilibrium Green's functions and the Wigner function.

The Wigner function is a real-valued but not necessarily positive definite quasi-distribution, representing a quantum generalization of Boltzmann distribution. The Wigner function formalism is attractive as it allows the expression of quantum dynamics in a phase-space formulation, directly comparable with the classical analogue, more intuitive compared with the more abstract density matrix and Green's function approaches. At the same time the Wigner equation can be augmented by a Boltzmann-like collision operator accounting for the process of decoherence.

Although the Wigner equation has been introduced in 1932, the first finite-difference based solver appears in the mid 1980s (see [1] for a review), and more efficient solvers have been developed nowadays [2–8]. We have to wait until the beginning of 2000, to have particle Monte Carlo (MC) solvers for the Wigner equation [9,10]. From that period up to now, several papers have been published on this subject (see [11] for a review) and, recently, very interesting device simulations have been provided [12,13].

In the realm of the particle Monte Carlo methods, we have focused ourselves on the so called *Signed Monte Carlo method* [14]. Here, the Wigner potential is treated as a scattering source which determines the electron-potential interaction, and consequently new particles with different signs are stochastically added to the system. Recently this method has also been be understood in terms of the Markov jump process theory [15–18], producing a class of new stochastic algorithms.

In this paper a thorough validation of one of these algorithms will be presented, by comparing the Wigner MC results with the Schrödinger equation solution in an already traditional benchmark experiment which consists of the interaction of a Gaussian wave packet with a rectangular potential barrier. The MC simulation data show an excellent quantitative agreement with the corresponding Schrödinger solution, with reasonable computational times.

2. The Signed particle Monte Carlo method

The Wigner equation has the form [19]

$$\frac{\partial}{\partial t} f_w(t,x,k) + \frac{\hbar}{m^*} k \cdot \nabla_x f_w(t,x,k) = \mathcal{Q}(f_w) \tag{1}$$

where $x \in \mathbb{R}^d$ is the particle position, $k \in \mathbb{R}^d$ the wave vector (and $\hbar k$ the momentum), m^* the particle mass, which includes the quantum evolution term

$$\mathcal{Q}(f_w) = \int V_w(x, k-k') f_w(t,x,k')\, dk' \tag{2}$$

where V_w is the Wigner potential

$$V_w(x,k) = \frac{1}{i\hbar(2\pi)^d} \int dx'\, e^{-ik\cdot x'} \left[V\left(x + \frac{x'}{2}\right) - V\left(x - \frac{x'}{2}\right) \right] \tag{3}$$

and $V(x)$ the potential energy. The Wigner potential is a non-local potential operator which is responsible of the quantum transport, is real-valued, and anti-symmetric with respect to k.

The solution $f_w(t,x,k)$ is real valued, but not necessarily nonnegative, and it is related to the solution $\psi(x,t)$of the Schrödinger equation. Under certain hypothesis on the $\psi(x,t)$, the function $f_w(t,x,k)$ satisfies

$$n_q(x,t) = \int f_w(t,x,k)\, dk = |\psi(x,t)|^2 \geq 0. \tag{4}$$

Solving the Wigner equation, from the numerical point of view, is a quite difficult task. The main complication arising in the direct solution based on finite-difference scheme, is the discretization of the diffusion term $k \cdot \nabla_x f_w$ due to the typically fast variation in the phase space. Particle based MC techniques do not require the discretization of this term, but they need costly computational times.

In the following we shall follow the so called *Signed particle Monte Carlo approach* developed initially in [14]. This technique is based on the observation that the quantum evolution term (2) looks like the *Gain* term of a collisional operator in which the *Loss* term is missing. But the Wigner potential (3) is not always positive and cannot be considered a scattering term. For this reason, it can be separated into a positive and negative parts V_w^+, V_w^- such that

$$V_w = V_w^+ - V_w^- \quad , \quad V_w^+, V_w^- \geq 0 \quad . \tag{5}$$

In this way, we can define an integrated scattering probability per unit time as

$$\gamma(x) = \int dk'\, V_w^+(x, k-k') = \int dk'\, V_w^-(x, k-k') \tag{6}$$

and rewrite the quantum evolution term as the difference between *Gain* and *Loss* terms, i.e.

$$\mathcal{Q}(f_w) = \int dk' w(k',k) f_w(t,x,k') - \gamma(x) f_w(t,x,k) \tag{7}$$

$$w(k',k) = V_w^+(x, k-k') - V_w^-(x, k-k') + \gamma(x)\delta(k-k') \quad . \tag{8}$$

Now the term $w(k',k)$ is interpreted as a new scattering rate which produces, from the old particle, a new pair of particles having weight (or Affinity) A and $-A$. In conclusion, an initial parent particle (with sign) evolves on a free-flight trajectory and, according to a generation rate given by the function $\gamma(x)$, two new signed particles are generated in the same position having weight A and $-A$ respectively. The momentum of the new particles is generated with probability $V_w^+(x,k)/\gamma(x)$.

However this procedure suffers from many drawbacks such as: efficiency issue in particle generation, because γ usually is a rapidly oscillating function, and exponential growth of particle numbers. In order to contain the particle number, a cancellation procedure must be introduced in such a way that, if the total number of particles exceeds a certain bound N_{canc}, then pairs of particles with similar positions and wave vectors, but with opposite signs, are removed from the system.

3. The no-splitting algorithm

The previous creation process has been understood in terms of the Markov jump process theory. The particle system is characterized by the state space

$$z_j(t) = (A_j(t), x_j(t), k_j(t)), \quad t \geq 0 \quad , \quad j = 1, .., N(t) \tag{9}$$

where the first component is the weight $A_j \in \{-1, +1\}$, the second component is the position vector, and the third component is the wave-vector. The time evolution of the system is determined by the flow

$$F(t, z) = (A, x + v(k)t, k) \quad , \quad v(k) = \frac{\hbar k}{m^*}$$

and a jump kernel $\lambda(z)$. The random waiting time τ until the next jump satisfies

$$\mathbb{P}(\tau \geq t) = \exp\left\{ - \int_0^t \lambda(F(s, z))\, ds \right\} \quad . \tag{10}$$

In our case the jump is the creation of a pair whose creation rate and the offspring distribution are determined by the kernel λ. It is possible to prove that this piecewise deterministic Markov jump satisfies a weak form of the Wigner equation [15], and some examples of creation kernel are given in [16]. In particular, we have considered the creation procedure which uses an upper bound of the Wigner potential, i.e.

$$|V_w(x, k)| \leq \hat{V}_w(x, k) \quad \forall x, k, \in \mathbb{R}^d \tag{11}$$

and, in this case, we have (see [18] for details)

$$\lambda(F(s, z)) = \sum_{j=1}^{N} \hat{\gamma}(x_j + v(k_j)s) \quad , \quad \hat{\gamma}(x) = \frac{1}{2} \int_{\mathbb{R}^d} \hat{V}_w(x, k)\, dk \quad . \tag{12}$$

If we substitute eq.(12) into eq.(10), due to the complexity of the integral in the exponent, it is impractical to generate stochastic waiting times τ and, for this reason, a time-splitting procedure must be introduced, producing a time-step error. But if $\hat{\gamma}(x)$ does not depend on x, i.e. it is constant, we have

$$\mathbb{P}(\tau \geq s) = \exp\left(- \int_0^s \hat{\gamma} N ds \right) = \exp\left(-\hat{\gamma} N s\right) \rightarrow \quad \tau = -\frac{1}{\hat{\gamma} N} \log r$$

where $r \in U(0, 1)$ is a uniform random number, and the random waiting time τ is completely determined. In this case, a new no-splitting generation algorithm has been introduced in [18] without time discretization error, which will be validated with a well-known benchmark model in the next section.

4. The rectangular barrier benchmark

The benchmark test we choose for the validation of the no-splitting generation algorithm, consists of the interaction of a Gaussian wave packet with a one dimensional rectangular potential barrier. The one dimensional potential barrier is

$$V(x) = a\, \chi_{[-b/2, b/2]}(x) \quad , x \in \mathbb{R} \tag{13}$$

and the corresponding Wigner potential is

$$V_w(x, k) = \frac{2a}{\hbar \pi k} \sin(2kx)\, \sin(kb) \quad x, k \in \mathbb{R} \quad . \tag{14}$$

The upper bound (11) is

$$\hat{V}_w(x, k) = \frac{2ab}{\hbar \pi} \quad , \quad \hat{\gamma} = \frac{2abc}{\hbar \pi} \tag{15}$$

where c is a cutoff in k in the integral (12). The initial condition for the Wigner equation is

$$f_w(0,x,k) = \frac{1}{\pi\sigma_0^2}\exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right]\exp\left[-2(k-k_0)^2\sigma_0^2\right] \tag{16}$$

where x_0 = -6 nm, k_0= 0.46 nm^{-1}, σ_0 = 1 nm, which it is plotted in figure 1 whereas in figure 2 the corresponding mean density (4) is shown. The height and width of the potential barrier (13) are

$$a = 0.3\,\mathrm{eV} \quad , \quad b = 2.14\,\mathrm{nm} \quad . \tag{17}$$

In the x-space we have considered an uniform mesh [-20, 20](nm) with $N_x = 200$ grid-points; also in the k-space we have an uniform mesh [-7.78, 7.78](nm^{-1}) with N_k=256. We have chosen absorption boundary conditions, i.e. if a particle is out of the mesh then it is erased. The cutoff has been fixed $c = 7.68$ nm^{-1}, the initial particle number is $N_{ini} = 160000$, the cancellation parameter $N_{canc} = 480000$.

Since for a pure state the Wigner and Schrödinger equations are equivalent, we shall compare the MC results with the corresponding analytic solution of the Schrödinger equation found by Los et al. [20]. The initial condition for the Schrödinger equation is

$$\psi(x,0) = \frac{1}{(2\pi\sigma_0^2)^{\frac{1}{4}}}\exp\left[-\frac{(x-x_0)^2}{4\sigma_0^2}\right]\exp(ik_0x) \quad . \tag{18}$$

In the figures 3-10 we show the Wigner distribution function $f_w(t,x,k)$ and the corresponding mean density (4), for some values of the simulation time. The mean density plots show no visible deviation of the MC numerical approximation from the analytic curve.

The CPU time for the no-splitting algorithm was 435 sec., which is considerable smaller than the CPU time consumed by a splitting-based algorithm (3929 sec.). The results presented have been obtained using an AMD Phenom II X6 1090T 3.2GHz and 8 Gb RAM.

5. Conclusions

The Wigner equation has been solved by using the Signed particle Monte Carlo method, where a new pair of particles characterized by a sign are created randomly and added to the system. This creation mechanism has been recently interpreted in terms of the Markov jump process, producing a class of new stochastic algorithms [16]. One of these algorithms has been implemented without time discretization error, and it has been applied to the rectangular potential barrier benchmark. The results are compared with the corresponding analytic solution for the Schrödinger equation, showing an excellent agreement as well as a low-cost computational effort. Future researchers will develop this MC methodology for the simulation of realistic devices, such as silicon nanowires according to the guidelines in [21–25].

Acknowledgment

We acknowledge the support of the project "Modellistica, simulazione e ottimizzazione del trasporto di cariche in strutture a bassa dimensionalità", Università degli Studi di Catania - Piano della Ricerca 2016/2018 Linea di intervento 2.

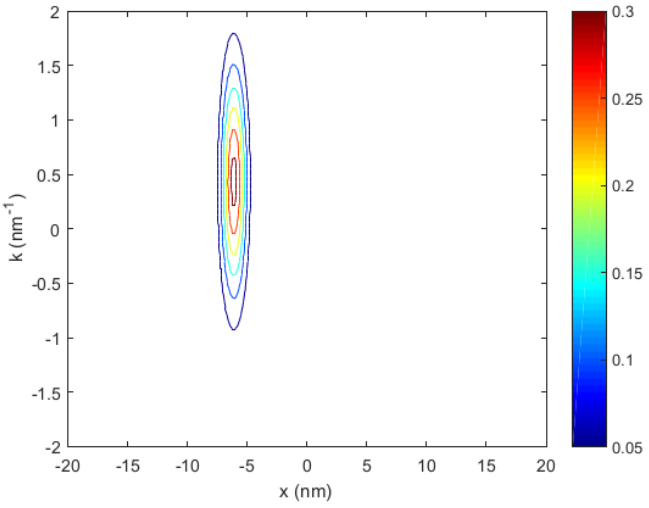

Figure 1. Wigner distribution function $f_w(x,k,t)$ at t = 0 fsec.

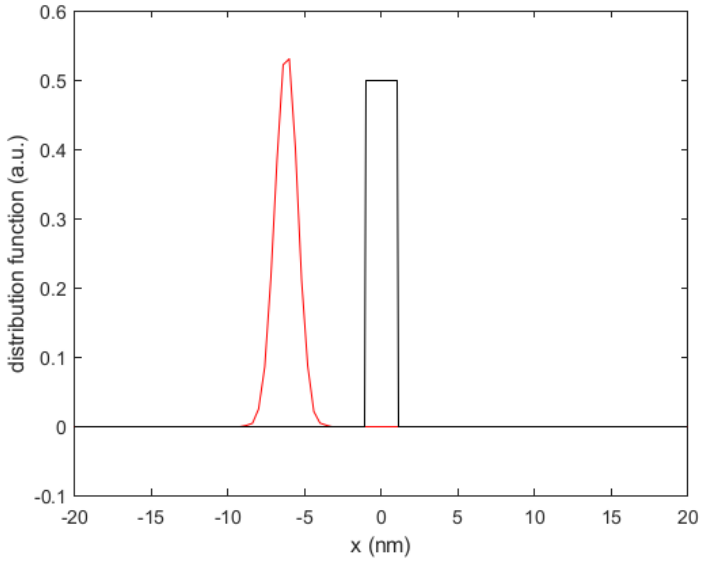

Figure 2. Mean density (4) versus position at t = 0 fsec.

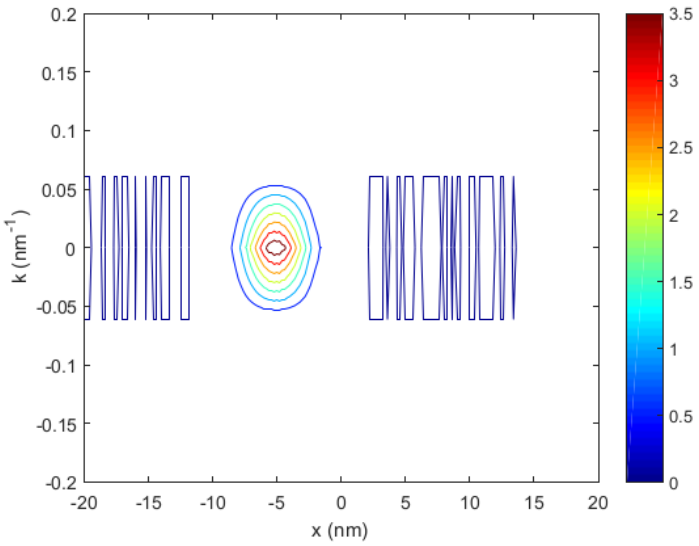

Figure 3. Wigner distribution function $f_w(x, k, t)$ at t = 6 fsec.

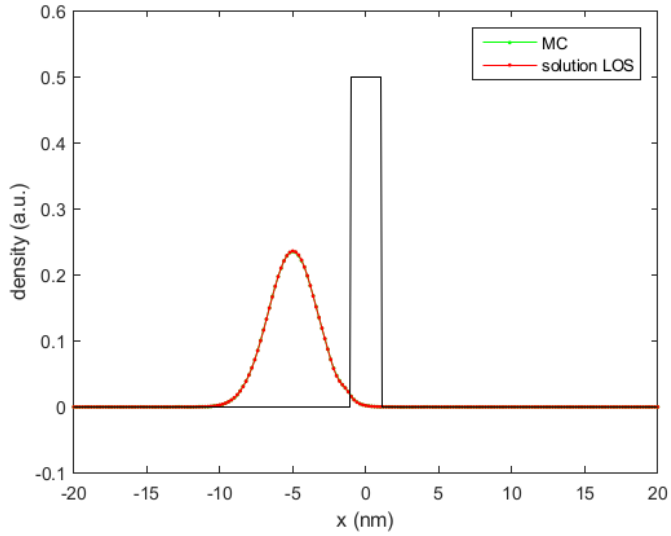

Figure 4. Mean density (4) versus position for t = 6 fsec., obtained with MC simulation and the corresponding analytic solution of the Schrödinger equation [20].

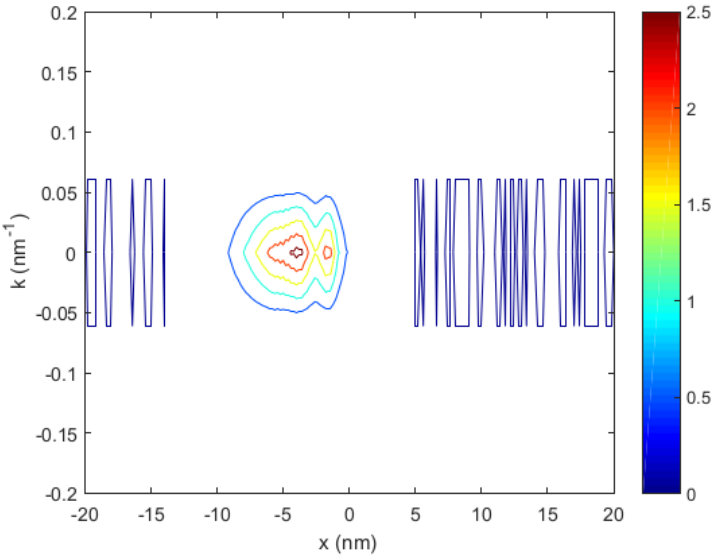

Figure 5. Wigner distribution function $f_w(x,k,t)$ at t = 10 fsec.

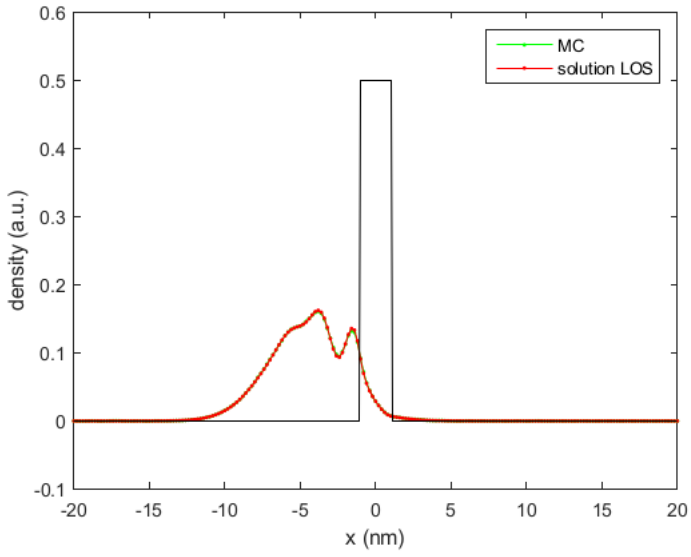

Figure 6. Mean density (4) versus position for t = 10 fsec., obtained with MC simulation and the corresponding analytic solution of the Schrödinger equation [20].

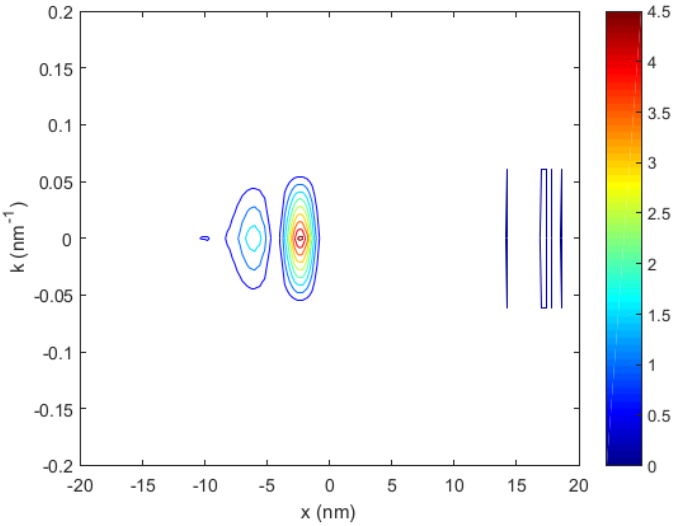

Figure 7. Wigner distribution function $f_w(x, k, t)$ at t = 20 fsec.

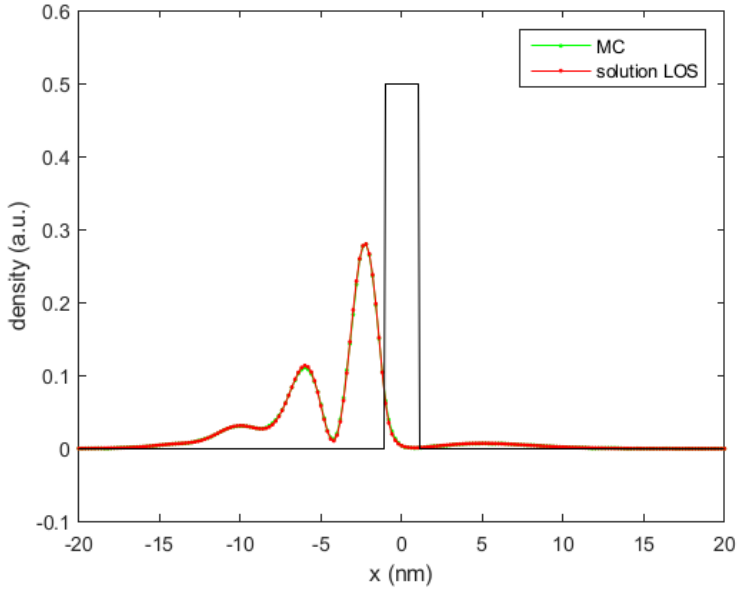

Figure 8. Mean density (4) versus position for t = 20 fsec., obtained with MC simulation and the corresponding analytic solution of the Schrödinger equation [20].

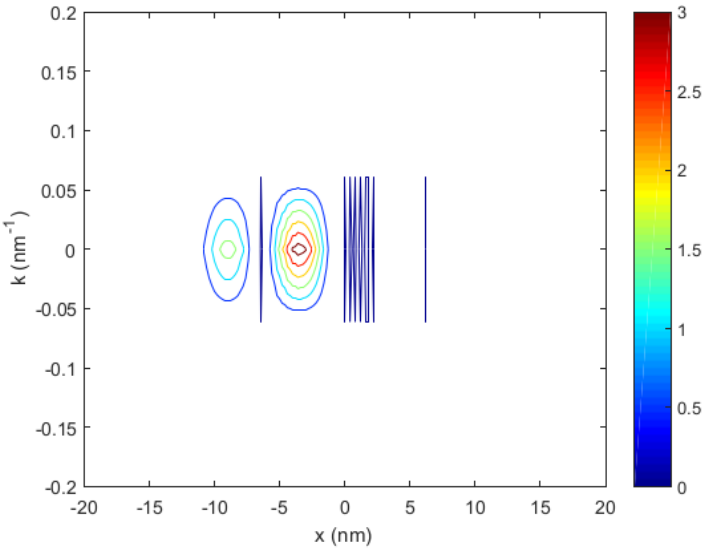

Figure 9. Wigner distribution function $f_w(x, k, t)$ at t = 30 fsec.

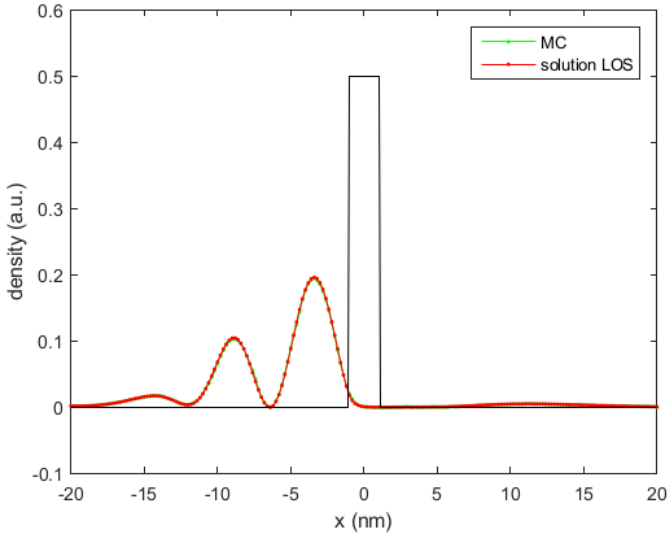

Figure 10. Mean density (4) versus position for t = 30 fsec., obtained with MC simulation and the corresponding analytic solution of the Schrödinger equation [20].

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