Optimized Particle Regeneration Scheme for the Wigner Monte Carlo Method

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Abstract. The signed-particle Monte Carlo method for solving the Wigner equation has made multi-dimensional solutions numerically feasible. The latter is attributable to the concept of annihilation of independent indistinguishable particles, which counteracts the exponential growth in the number of particles due to generation. After the annihilation step, the particles regenerated within each cell of the phase-space should replicate the same information as before the annihilation, albeit with a lesser number of particles. Since the semi-discrete Wigner equation allows only discrete momentum values, this information can be retained with regeneration, however, the position of the regenerated particles in the cell must be chosen wisely. A simple uniform distribution over the spatial domain represented by the cell introduces a 'numerical diffusion' which artificially propagates particles simply through the process of regeneration. An optimized regeneration scheme is proposed, which counteracts this effect of 'numerical diffusion' in an efficient manner.

1 Introduction

The Wigner formalism expresses quantum mechanics, which normally is formulated with the help of wave functions and operators, in terms of functions and variables defined in the phase-space. This reformulation in the phase-space facilitates the reuse of many classical concepts and notions.

The Wigner transform of the density matrix operator yields the Wigner function, $f_w(x,p)$, which is often called a quasi-probability function as it retains certain properties of classical statistics, but suffers of negative values. The associated evolution equation for the Wigner function follows from the von Neumann equation for the density matrix, which for the illustrative, one-dimensional case is written as

$$\frac{\partial f_w}{\partial t} + \frac{p}{m^*}\frac{\partial f_w}{\partial x} = \int dp' V_w(x, p-p')\, f_w(x,p',t)\,. \tag{1}$$

If a finite coherence length is considered – the implications and interpretation of which is discussed in [2,5] – the semi-discrete Wigner equation results and the momentum values are quantized by $\Delta k = \pi/L$ and the integral is replaced by a summation. Henceforth, the index q refers to the quantized momentum, i.e. $p = \hbar(q\Delta k)$.

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Equation (1) is reformulated as an adjoint integral equation (Fredholm equation of the second kind) and is solved stochastically using the particle-sign method [4]. The latter associates a + or – sign to each particle, which carries the quantum information of the particle. Furthermore, the term on the right-hand side of (2) gives rise to a particle generation term in the integral equation; the statistics governing the particle generation are given by the Wigner potential (i.e. the kernel of the Fredholm equation), which is defined here as

$$V_w(x,q) \equiv \frac{1}{i\hbar L}\int_{-\mathbf{L}/2}^{\mathbf{L}/2} ds\, e^{-i2q\Delta k\cdot s}\left\{V(x+s)-V(x-s)\right\}. \tag{2}$$

A generation event entails the creation of two additional particles with complementary signs and momentum offsets q' and q'', with respect to the momentum q of the generating particle. The two momentum offsets, q' and q'', are determined by sampling the probability distributions $V_w^+(x,q)$ and $V_w^-(x,q)$, dictated by the positive and negative values of the Wigner potential in (2), respectively:

$$V_w^+(x,q) \equiv \max(0,\, V_w); \tag{3}$$

$$V_w^-(x,q) \equiv \min(0,\, V_w). \tag{4}$$

The generation events occur at a rate given by

$$\gamma(x) = \sum_q V_w^+(x,q), \tag{5}$$

which typically lies in the order of $10^{15}s^{-1}$. This rapid increase in the number of particles makes the associated numerical burden become computationally debilitating, even for simulation times in the order of femtoseconds.

The notion of particle annihilation is used to counteract the exponential increase in the number of particles, due to particle generation. This concept entails a division of the phase space into many cells – each representing a volume $(\Delta x\Delta k)$ of the phase space – within which particles of opposite sign annihilate each other: Consider a cell (i,q) within the phase-space, which encompasses all particles with a momentum of $\hbar\,(q\Delta k)$ and a position within the spatial domain $\Omega_i = [x_i,\, x_i+\Delta x]$. The particles within the cell are considered identical and indistinguishable, i.e. any positive particle may annihilate any negative particle in the cell and vice versa. Within the cell (i,q), let there be P_i particles with a positive sign and Q_i particles with a negative sign which are summed up to yield a remainder of particles, $R_i = P_i - Q_i$; $|R_i|$ particles, each carrying the sign of R_i, are regenerated within the cell.

The $|R_i|$ particles that survive the annihilation procedure should, ideally, replicate the same distribution in cell (i,q) as represented by the (P_i+Q_i) particles before the annihilation step. Since the momenta are quantized and a single value is shared amongst all particles within a cell, the distribution in the k-space can be recovered after annihilation. The positions of the particles, however, are real-valued, which prompts a closer inspection of the regeneration process to retain this information.

2 Particle Regeneration Schemes

The straight-forward approach to regeneration – leaning on the assumption of identical, indistinguishable particles used for the annihilation – would be to spread the $|R_i|$ particles uniformly in space, over the domain Ω_i. This approach, however, leads to a 'numerical diffusion' of particles, which causes the global particle ensemble to propagate at a different rate than dictated by its k-distribution. The evolution of a minimum uncertainty wave packet, defined as

$$f_w(x,k) = \mathcal{N}^{-\frac{(x-x_0)^2}{\sigma^2}} e^{-(k-k_0)^2\sigma^2}, \tag{6}$$

with $x_o = -50\,\mathrm{nm}$, $k_0 = 6\left(\frac{\pi}{50}\right)\mathrm{nm}^{-1}$ and $\sigma = 10\,\mathrm{nm}$, is compared in Fig. 1 using three different approaches: (i) an analytical solution, (ii) a Monte Carlo approach without any re-generation and (iii) a Monte Carlo approach with a (forced) regeneration procedure at each time step. A typical time step, for simulations in which annihilation is required due to particle generation, of 0.1 fs is chosen. It is evident that approaches (i) and (ii) correspond exactly, however, the wave packet which is subjected to the regeneration procedure spreads out faster. This discrepancy is solely due to the regeneration procedure and is analyzed in the following.

Consider an ensemble of N particles, with positions $\{p_j\}$ $j = 1 \ldots N$, $p_j \,\epsilon\, \Omega_i$, within the cell (i,q) at time t_0. The mean position of the ensemble at time t_0 is

$$\begin{aligned}\bar{p}_0 &= \frac{1}{N}\sum_{j=1}^{N} p_j \\ &= x_i + \frac{1}{N}\sum_{j=1}^{N} \delta x_j,\end{aligned} \tag{7}$$

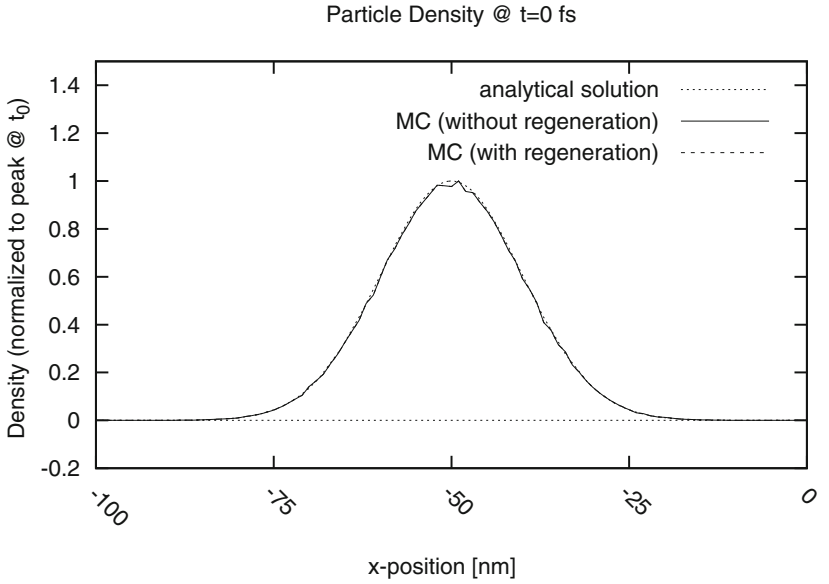
where the position is expressed as $p_j = x_i + \delta x_j$, $\delta x_j \,\epsilon\, [0, \Delta x]$. The particles of the ensemble evolve (drift) for a time period Δt, whereafter the mean position of the ensemble at time t_1 is

$$\begin{aligned}\bar{p}_1 &= \frac{1}{N}\sum_{j=1}^{N} p_j + v_j \Delta t \\ &= x_i + \frac{1}{N}\sum_{j=1}^{N} \delta x_j + v_j \Delta t,\end{aligned} \tag{8}$$

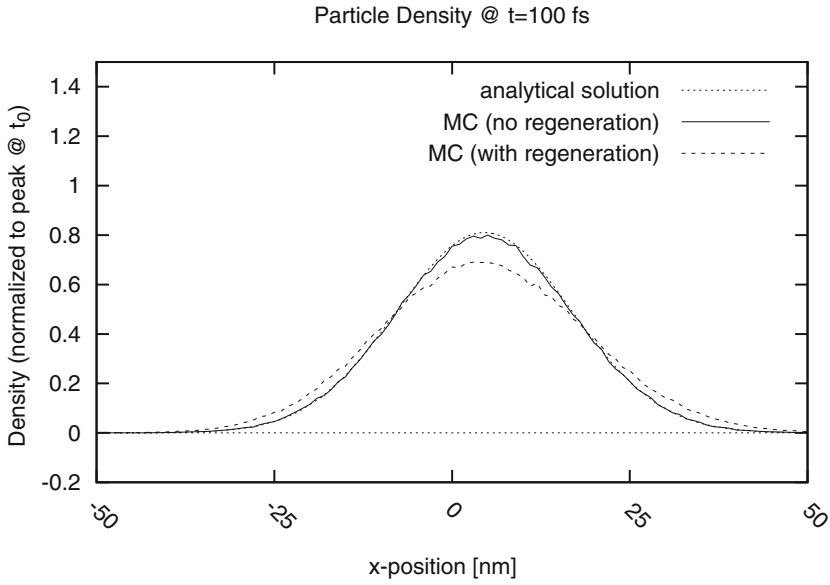
where v_j denotes the velocity of particle j, which is assumed to be small enough such that the particle remains within the bounds of the cell for one time step. Since we only have a single discrete momentum value associated with the cell, the velocity of all particles within the cell is the same (v_m). Therefore,

$$\bar{p}_1 = \bar{p}_0 + v_m \Delta t. \tag{9}$$

Now, suppose that before the particle evolution commences an annihilation step is performed, whereafter N' particles are regenerated within the cell with positions



(a)



(b)

Fig. 1. Comparison of a wave packet evolved from (a) 0 fs to (b) 100 fs, using an analytical solution and a Monte Carlo (MC) approach without and with the regeneration process (repeated every 0.1fs).

$\{p'_j\}$ $j = 1 \ldots N' \leq N$. If the particles are uniformly distributed over the cell, one imposes

$$\bar{p}'_0 = \frac{x_i + x_{i+1}}{2} = x_i + \frac{\Delta x}{2}. \tag{10}$$

Consequently, the mean position of the ensemble at time t_1 will be

$$\bar{p}'_1 = x_i + \frac{\Delta x}{2} + v_m \Delta t, \tag{11}$$

which, when compared to (9), introduces an artificial propagation/retardation depending on the spatial distribution of particles before the annihilation procedure.

The original spatial distribution of the particles within a cell can be perfectly recovered, if all (infinitely many) of the moments of the distribution before the annihilation are known (and the Carleman's condition [1] for uniqueness is satisfied). The mean position represents the first moment of the local distribution and already retains the most important information. By uniformly distributing the particles over a distance Δx around the pre-annihilation mean, the 'numerical diffusion' is effectively remedied, albeit with some added 'noise', as shown in Fig. 2. This 'noise' is attributed to the fact that the uniform distributions of neighbouring cells overlap.

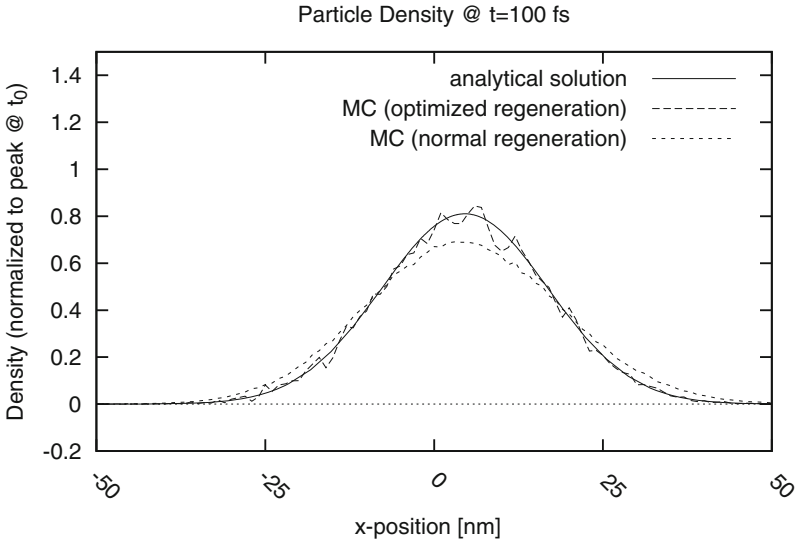


Fig. 2. Comparison of wave packets evolved for 100 fs using an optimized regeneration scheme and the conventional regeneration process; analytical solution shown by the solid line.

If, in addition to the mean, the second moment of the distribution – the standard deviation – is also calculated the particles can be regenerated using e.g. a

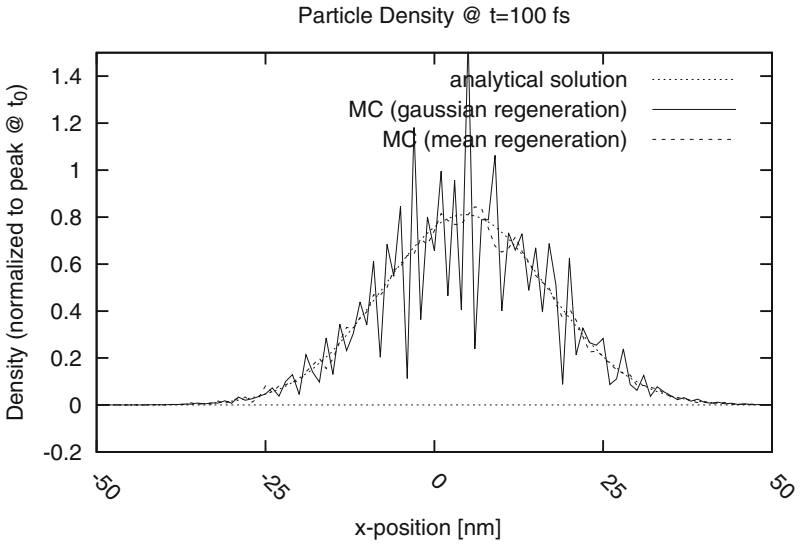


Fig. 3. Comparison of wave packets evolved for 100 fs using regeneration schemes based on a Gaussian distribution and a mean with uniform distribution (as in Fig. 2); the analytical solution is shown for comparison.

Gaussian distribution. The result, shown in Fig. 3, is very noisy, however, since a Gaussian distribution poorly models the actual distribution in each cell in this specific case and concentrates most of the particles in cell in a small region. The quality of the regenerated distribution may be refined indefinitely, by considering more moments of the distribution. While the increase in computation time required to calculate additional moments remains almost negligible (<1 % for the presented cases), to recover a distribution from (some of) its moments – the so-called Classic Moment Problem [1,6] – is quite challenging.

A flexible distribution, like the generalized Lambda distribution (GLD) [3], which can assume a wide variety of shapes is well-suited to describe an arbitrary distribution quite accurately. The GLD is defined using four parameters which are based on the first four moments of the distribution and solving up to four nonlinear equations, making the computational effort high, if this process must be repeated for each cell in the phase space. Therefore, the computational costs should be weighed against the gained advantages and other techniques, like simply decreasing Δx.

3 Conclusion

It has been shown that an artificial propagation/retardation of particles arises when solving the semi-discrete Wigner equation, using the signed-particle method. This 'numerical diffusion' arises, if the particle regeneration process does not consider the spatial distribution of particles, within a phase-space cell, prior to

annihilation. Calculating the mean value of the particles within a cell – the first moment of the distribution – before regenerating them has emerged as an efficient approach to counteract the 'numerical diffusion'. Fitting the distribution using more moments is not trivial and incurs considerable computational costs.

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