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# Absorbing-like boundaries for quantum field theoretical grid simulations

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ABSTRACT

We introduce a computational method that permits us to increase the interaction time for quantum mechanical and quantum field theoretical simulations of multi-particle states on a finite space–time grid. In contrast to the usual approach where the unwanted portion of the wave function close to the grid boundaries is absorbed by a potential with a negative imaginary part, this method is unitary and therefore conserves the norm of the state. This technique is based on assigning particles close to the boundary a larger effective mass (or slower speed of light) such that the particles slow down and cannot re-enter the interaction zone. The method can therefore be applied to multi-particle states for which imaginary potential methods fail.



## 1. Introduction

Space–time resolved simulations of the evolution of quantum wave packets in various external fields have greatly advanced our knowledge of dynamical systems in atomic, molecular, optical and chemical physics. In these numerical solutions to the time-dependent Schrödinger or Dirac equation, the spatial coordinate axes are usually discretized into a finite number of grid points and the time-evolution is obtained iteratively. The maximum interaction time that can be studied is then limited by the finite length of the numerical box. Once portions of the wave packet that normally would escape to infinity reach the edges of this box, they are either reflected or wrapped around to the other edge, depending on the boundary conditions. These portions can then re-enter the interaction region, which leads to unwanted and unphysical interferences. Extending the numerical size of this box is often not practical due to restrictions on computer memory as well as CPU time.

In order to compensate for these unwanted portions of the wave packet and therefore to extend the interaction time, several proposals have been made [1–7]. They include the introduction of a potential with a negative imaginary part, which is equivalent to applying a masking function, as well as complex coordinate rotation or exterior complex scaling [8–12], and complex spatial variables have also been examined for single particle systems. For example, these methods have been applied to study the generation of higher-harmonics in ionization [13] and double-ionization in strong-field physics [14].

In the last few years the space–time resolved approach has also been generalized to simulate the dynamics of quantum field theoretical systems, but the interaction time is again restricted by the same bottleneck as particle densities reach the boundaries [15]. In this case the above techniques are not applicable. In this note we discuss a new unitarity-preserving computational method to increase the interaction time. Instead of removing the unwanted portions of the spatial density that have reached the boundary, they are assigned a larger mass (or a smaller speed of light), leading to an effective slow-down ("parking") of density in this particular region. In this way, the particles are prohibited from re-entering the interaction zone. We discuss below how to optimize these parking zones for specific quantum mechanical and quantum field theoretical model systems.

## 2. Difficulties associated with the non-unitary evolution of multi-particle systems

As mentioned in the Introduction, the inclusion of an extra negative imaginary potential close to the boundary regions can extend the interaction time of single-particle wave packet simulations significantly. For example, a constant negative imaginary part would lead to a spatially exponential decay of the wave function. The optimum choice for the spatial profile of such a potential is determined by the three competing requirements to (1) minimize the number of spatial grid points that are allocated to represent the absorbing

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spatial region, (2) to maximize the degree of absorption and (3) to minimize the reflection due to this potential itself. The second point can be accomplished by increasing the amplitude of the potential and its spatial extension. The reflection can be minimized if the amplitude of the potential is not too large and if it is slowly ramped up over a sufficiently large spatial domain.

For a single-particle wave function, $\Psi(x,t) = \psi_1(x,t) + \psi_2(x,t)$, where $\psi_1(x,t)$ is localized in the interaction region and $\psi_2(x,t)$ is localized near the boundary, this method works very well, as only the unwanted portion $\psi_2(x,t)$ (which has reached the absorbing zone) is simply removed from the state, which effectively reduces the norm of the remaining state $\Psi(x,t) = \psi_1(x,t)$. Ideally, we would like to generalize this technique to simulations that describe more than just one particle and "remove" only that particular particle from the simulation that has approached the grid edge. To illustrate this for a simple example, let us assume that we have the simplest case of an (uncorrelated) two-particle wave function $\Psi(x,y,t) = \psi_1(x,t)\psi_2(y,t)$, where the second particle described by the state $\psi_2(y,t)$ has reached the absorbing zone. Unfortunately, an imaginary potential $V(x,y)$ is not able to differentiate between $\psi_1(x,t)$ and $\psi_2(y,t)$ and would therefore reduce the norm of the *entire* state $\Psi(x,y,t)$. An ideal and truly discriminating absorption mechanism would be able to "remove" only the unwanted portion of $\psi_2(y,t)$ from $\Psi(x,y,t)$, therefore effectively reducing a two-particle state into a single-particle state characterized solely by $\psi_1(x,t)$. Unfortunately, this reduction of the total number of particles cannot be accomplished within a quantum mechanical calculation.

In the framework of quantum field theory, however, a reduction from a two- to a single-particle system could be modeled, in principle, but it is not practical due to the occurrence of unwanted interferences as we will discuss below. In fact, it is not possible within a wave function based formalism to reduce an initial two-particle state $|2\rangle$ to a one-particle state $|1\rangle$ without the occurrence of unavoidable interferences as the state $|1\rangle$ is built up continuously in time.

To have the simplest possible model system [16] to illustrate this effect, let us assume that the state is given by the superposition $|\Psi(t)\rangle = C_1(t)|1\rangle + C_2(t)|2\rangle$ and the continuous removal of the unwanted particle at the boundary is modeled by the (non-Hermitian) Hamiltonian, $H = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2| + |1\rangle\langle 2|$, where for simplicity all single and two-particle energies are lumped together as $E_1$ and $E_2$, respectively. In this Hamiltonian the population can flow only to the single-particle state $|1\rangle$, but not to $|2\rangle$, as it does not contain a coupling $|2\rangle\langle 1|$. The resulting equations of motion of the amplitudes, $i\,dC_1/dt = E_1C_1 + C_2$ and $i\,dC_2/dt = E_2C_2$, can be easily solved for $|\Psi(t=0)\rangle = |2\rangle$, leading to $C_1(t) = [\exp(-iE_2t) - \exp(-iE_1t)]/(E_2 - E_1)$ and $C_2(t) = \exp[-iE_2\,t]$. The time evolution of the population of the single-particle state is simply given by $|C_1(t)|^2 = [2\sin[t(E_2 - E_1)/2]/(E_2 - E_1)]^2$. After the expected initial growth of $|C_1(t)|^2$, at a characteristic time $t = \pi/(E_2 - E_1)$ this probability begins to decay again, even though the Hamiltonian was purposely chosen to not contain any coupling term (such as $|2\rangle\langle 1|$) that could add a particle to the dynamics and therefore effectively decrease $|C_1(t)|^2$. The observed decrease of $|C_1(t)|^2$ can be understood in terms of a changing phase of the excitation associated with the time evolving state $C_2(t)|2\rangle$. At later times the state $|2\rangle$ takes a different phase than at earlier times; therefore, a destructive interference can lead to the decay in population in state $|1\rangle$. This decay is obviously a purely quantum mechanical mechanism that does not have any classical mechanical counterpart. In any case, this interference is unavoidable if one of the two particles is absorbed and therefore a single-particle state is created.

As a side note we might mention that an interference-free reduction from $|2\rangle$ to $|1\rangle$ can be described within a density matrix formalism and a corresponding master equation [17], but then the final state can no longer be described by a (coherent) wave function. Also, a density matrix would require a much larger Hilbert space than a state and therefore cannot really simplify a space–time grid simulation.

## 3. The parking scheme for the non-relativistic quantum mechanical evolution

### 3.1. The position-dependent mass $M(x)$

Before we discuss the quantum mechanical and field theoretical implementation, let us briefly consider the parking method from classical non-relativistic and relativistic perspectives. The main idea is to slow down the particle close to the boundary (in the parking zone) by assigning it a position-dependent mass, $M(x)$. Once the particle enters the zone, it slows down and increases the time it takes to hit the physical boundary without changing the norm of the state or the number of particles.

In order to describe the position dependent mass in terms of non-relativistic classical mechanics, we use the Hamiltonian formalism, where the Hamilton function is given by $h = p^2/(2M(x))$. We note that this formalism is equivalent to a Newtonian formalism, where the analogue of Newton's 2nd law would read as $M(x)\,d^2x/dt^2 = -(dx/dt)^2\,(dM/dx)/2$. Of course, as h is time-independent, this leads to the conservation of the total energy, $E = p^2/[2M(x)]$.

For a mass function $M(x)$ that increases monotonically with $x$ inside the parking zone, the particle's momentum $p$ increases as its velocity decreases for the non-relativistic quantum mechanical discussion below. This follows directly from conservation of the total energy, which also shows that $p/M(x)$ decreases with increasing $x$. During the entire evolution, the velocity $dx/dt = \partial h/\partial p = p/M(x)$ decreases but remains positive, while $dp/dt = -\partial h/\partial x = (1/2)p^2/M(x)^2\,dM/dx$ is always positive. We also note that the particle can only come to a complete halt if the mass function $M(x)$ has a singularity and becomes infinite. Take the simple example of a linearly ramped-up mass, $M(x) = m[1 + \alpha(x - x_M)\theta(x - x_M)]$, where $\theta(\cdots)$ denotes the Heaviside unit step function, $x_M$ the beginning of the parking zone and $\alpha$ the potential strength. If a particle (with mass $m$) enters the zone at $t = 0$ with velocity $v$, we obtain $x(t) = x_M + [-1 + (1 + 3v\alpha t/2)^{2/3}]/\alpha$, which shows that the particle slows but does not stop in a finite distance, as $x(t) \sim t^{2/3}$ for long times.

In contrast to the non-relativistic limit, a relativistic particle, modeled by $h = [M(x)^2c^4 + c^2p^2]^{1/2}$ can come to rest at a *finite* distance $x$ even if the mass function is not singular. We denote with $c$ the speed of light, and from now on we use atomic units where $c = 137.036$. This finiteness follows from energy conservation, which prohibits an incoming particle with true mass $m$ from visiting spatial regions that are associated with an energy larger than $E = [m^2c^4 + c^2p_0^2]^{1/2}$, where $p_0$ is its initial momentum. In other words, a relativistic orbit cannot exceed $x_{\lim}$, defined by $M(x_{\lim}) = [m^2 + c^{-2}p_0^2]^{1/2}$. Furthermore, its canonical momentum $p$ decreases as a function of time, as $dp/dt = -c^4M(x)dM/dx/h$ is always negative. As a result, in contrast to the non-relativistic case, the particle can turn around and return to the interaction zone, which is undesirable. This is also obvious from the non-relativistic limit ($c \to \infty$) of the Hamilton function $h$, where the leading terms play the role of an extra potential, $h = M(x)c^2 + p^2/[2M(x)] + O[(p/c)^4]$. As a concrete example, if we again ramp up the mass linearly, $M(x) = m[1 + \alpha(x - x_M)\,\theta(x - x_M)]$, we would obtain $x_{\lim} = x_M + [(1 + p_0^2m^{-2}c^{-2})^{1/2} - 1]/\alpha$.

### 3.2. The optimization of the mass function $M(x)$ in the non-relativistic case

An implementation of the parking mechanism in a non-relativistic quantum simulation is rather straightforward and can