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Split-operator technique for propagating phase space functions: Exploring chaotic, dissipative and relativistic dynamics

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ABSTRACT

We conduct a comprehensive analysis of the split-operator method for propagating phase space distribution functions in different scenarios of classical mechanics. A numerical method based on Fast Fourier Transform allows to propagate almost any sampled or exact localized initial state, as well as the direct calculation of current densities in phase space. In order to demonstrate the potential of the proposed numerical scheme some simulations involving chaotic, dissipative and relativistic dynamics are performed. In the conducted simulations, dynamical functions like autocorrelations as well as the detailed structures in phase space are discussed. We find that the split-operator technique demonstrates the effectiveness for studying time evolution of interacting one-dimensional classical systems.

1. Introduction

The split-operator technique (SOT) has been considered one of the most plausible alternatives to perform the time-evolution of localized initial states in quantum systems. It has been successfully applied for the solution of the Schrödinger equation in coordinates as well as phase space representations [1–4]. It has become an ideal for propagating initial states in many branches of physics, for instance, applications involving wave-packet dynamics in molecular systems [5–7] and frequent use of quantum molecular dynamics [8,9]. In the recent past, Finite difference has adopted the SOT scheme to simulate propagation phenomena in quantum mechanics and quantum field theory [10,11]. Moreover, the versatility of this hybrid model becomes an advantage of using both modeling schemes; Noticeably, to simulate the scattering of sound in the time-dependent domain [12], and the propagation of waves through optical fibers [13]. Recently, the SOT has exploited the power of high performance computing and it has been implemented in modern hardware architectures for solving time-dependent Schrödinger equations and time-dependent Dirac equations [14] as well as the Klein–Gordon equation [15]. In contrast to quantum mechanics, little is known about the benefits of this approach in the context of classical mechanics, in fact, there is only one work in the literature where this issue has been addressed in detail. More precisely, the pioneering work of Dattoli et al. [16] has developed a numerical method based on SOT for propagating the Liouville equation, and it was successfully applied for the case of a one-dimensional Hamiltonian system. Nevertheless, the numerical approach has not been widely noticed in many significant situations of classical dynamics. Possibly, it is due to their work having a limitation of implementation, the initial state should be known in an exact form as an inevitable step to perform the propagation in phase space. Furthermore, the traditional propagation methods in classical mechanics continue being the favorites to propagate initial states, since they involve mainly three stages, namely: (i) the initial state is frequently sampled on phase space accordingly with a particular distribution function, (ii) the corresponding classical trajectories are propagated at final time using a numerical integrator for solving the classical equations of motion; thus, those propagated trajectories contribute to the final state. (iii) In general, the propagated state should be smoothed in a grid, since all classical trajectories contribute in a different way to each phase space point. This methodology is commonly used in classical molecular dynamics [17,18], semiclassical propagation of wave-packets and Wigner functions [19–21], as well as studies about quantum–classical correspondence where a comparison with classical calculations is necessary [22,23]. However, it is worth mentioning that some complications can arise in the traditional propagation methods, for instance, the sampling method cannot

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always cover completely the initial state, and the convergence of methods as well as the propagated state will be a compromise. The numerical integration generally is time consuming when non-linearities appear in the classical equations of motion, and the propagated state requires a lot of classical trajectories in order to obtain a good resolution in phase space.

The present paper is concerned with classical phase space propagation based on the split-operator technique, and one of the motivations of this work is to fill the knowledge gap on this isolated topic. In order to achieve this, we will adopt the SOT to different scenarios of classical (relativistic) mechanics involving; regular, chaotic motion, and dissipative dynamics, and subsequently, propagation in high-dimensional phase spaces. We propose a numerical method for propagating phase space distribution functions with several advantages in contrast to the traditional methods. More precisely, (i) our approach is directly based on computations on a grid of size $N \times N$ representing the whole phase space of classical systems, thus the resolution in phase space is defined at the beginning of the calculation, and it can be managed with the actual computational resources. (ii) The initial state should be storage on grid, but it can be computed in exact form or sampled as is done by the traditional methods, and finally (iii) the numerical propagation is accomplished by the fast Fourier transform where the computation method takes the order of $\mathcal{O}(N \log N)$ operations that will reduce significantly the computational cost of the numerical simulations.

This paper is organized as follows: Section 2 explains the theoretical background of propagation phase space distribution functions according to the Liouville equation, and the numerical solution based on fast Fourier transform. In Section 3 we describe the method for propagating Hamiltonian systems with δ-kick interaction. In Sections 4 and 5 is considered for the time evolution of phase space distribution functions for dissipative dynamics associated with the classical limit of non-Hermitian quantum systems, and relativistic systems, respectively. The Section 6 deal with the phase space propagation for an interacting one-dimensional classical systems. Finally, we conclude in Section 7.

2. Liouville equation and the numerical schema

The time-evolution of phase space distribution function for a one-dimensional system is governed by the Liouville equation

$$\frac{\partial \rho(q,p;t)}{\partial t} = \hat{L}\rho(q,p;t), \tag{1}$$

where $\rho(q,p;t)$ is the phase space distribution function and $\hat{L}$ is the Liouville operator. The latter is given by

$$\hat{L} = \left[\frac{\partial H}{\partial q}\frac{\partial}{\partial p} - \frac{\partial H}{\partial p}\frac{\partial}{\partial q}\right] \tag{2}$$

where H is the classical Hamiltonian function. The solution to Eq. (1) can formally be written as $\rho(q,p;t) = \hat{U}(t)\rho(q_0,p_0;0)$, where $\rho(q_0,p_0;0)$ is the phase space distribution function at initial time, and the evolution operator is given by $\hat{U}(t) = \exp\{t\hat{L}\}$. In order to incorporate the split-operator technique, we split the full time evolution into $\delta t = t/N$ time steps, then the propagation in phase space can be written as:

$$\rho_{n+1}(q,p) = \hat{U}(\delta t)\,\rho_n(q,p), \quad n = 0, 1, \ldots, N-1 \tag{3}$$

where $\rho_n(q,p)$ indicates the phase space distribution function at the n-th time step, and the short-time evolution operator reads

$$\hat{U}(\delta t) = \exp\left(\frac{\delta t}{2}\hat{L}_1\right)\exp(\delta t\,\hat{L}_2)\exp\left(\frac{\delta t}{2}\hat{L}_1\right), \tag{4}$$

together with

$$\hat{L}_1 = -\frac{\partial H}{\partial p}\frac{\partial}{\partial q}, \qquad \hat{L}_2 = \frac{\partial H}{\partial q}\frac{\partial}{\partial p}. \tag{5}$$

Let us define the application of exponential operators $\exp(\frac{\delta t}{2}\hat{L}_1)$ and $\exp(\delta t\hat{L}_2)$ on the phase space distribution function. It reads in terms of Fourier transform

$$\begin{aligned}
&\mathcal{F}_q\left\{\exp\left(\frac{\delta t}{2}\hat{L}_1\right)\rho(q,p)\right\} = \exp\left(\frac{i\pi pq\delta t}{m}\right)\mathcal{F}_q\{\rho(q,p)\},\\
&\mathcal{F}_p\left\{\exp(\delta t\hat{L}_2)\rho(q,p)\right\} = \exp\left(-2\pi ipV'(q)\delta t\right)\mathcal{F}_p\{\rho(q,p)\},
\end{aligned} \tag{6}$$

where $V'(q) = dV(q)/dq$ is the first order energy derivative, and $\mathcal{F}_{q,p}$ ($\mathcal{F}_{q,p}^{-1}$) denotes the Fourier (inverse Fourier) transform in position or momentum coordinates, respectively. Thus, this yields a short-time evolution operator given by

$$\begin{aligned}
\hat{U}(\delta t) = {}& \mathcal{F}_q^{-1}\exp\left\{\frac{i\pi pq\delta t}{m}\right\}\mathcal{F}_q\mathcal{F}_p^{-1}\\
&\times \exp\left(-2\pi ipV'(q)\delta t\right)\mathcal{F}_p\mathcal{F}_q^{-1}\exp\left\{\frac{i\pi pq\delta t}{m}\right\}\mathcal{F}_q.
\end{aligned} \tag{7}$$

Note that here, we have considered the classical Hamiltonian function written in a standard form *i.e* $H = p^2/2m + V(q)$. However, it is not completely necessary as we will show in Section 5 for the relativistic case, where the kinetic term is much more complicated than this.

2.1. Algorithm for propagating phase space distribution functions

A simple algorithm that we proposed for propagating the phase space distribution functions compressed the following steps. (i) The first step consists of accumulating the localized initial state on an extended numerical grid, which will determine the availability of phase space. (ii) To divide the full time propagation in δt short-time steps and apply the short-time evolution operator according to Eq. (7). Noting that the Fourier transform implied here consists of both position and momentum coordinates, respectively. Accordingly this will be multiplied by corresponding phases. (iv) In order to achieve the full time propagation, to repeat the previous step on the propagated phase space distribution function and continue with this procedure until reaching the final time. It is noteworthy to mention that this numerical method allows to propagate virtually any localized initial state, for instance for propagating random initial states.

3. Propagation of δ-kicked systems

In the literature, impulsively driven systems are often referred to δ-kicked systems, due to the fact that the duration of each impulse is infinitely small compared to the period of the unperturbed system. These systems have become an essential tool for studying many phenomena from both theoretical and experimental perspectives, for instance, one of the primary approaches is quantum chaos in cold atoms [24,25], which ensures that it can provide valuable insights into non-linear-Hamiltonian dynamics, as well as the classical–quantum correspondence [26,27]. Although δ-kicked systems have been widely studied in the framework of quantum mechanics, there is no study about numerical methods in classical mechanics to propagate localized initial states, and this is the first time that SOT has been applied for δ-kicked systems. For a more detailed analysis of the way that the system changes upon each impulse, we present a numerical implementation for propagating an initial state perturbed by δ-kick interaction. Let us consider a