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Semi-spectral method for the Wigner equation

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ABSTRACT

We propose a numerical method to solve the Wigner equation in quantum systems of spinless, non-relativistic particles. The method uses a spectral decomposition into $L^2(\mathbb{R}^d)$ basis functions in momentum-space to obtain a system of first-order advection–reaction equations. The resulting equations are solved by splitting the reaction and advection steps so as to allow the combination of numerical techniques from quantum mechanics and computational fluid dynamics by identifying the skew-hermitian reaction matrix as a generator of unitary rotations. The method is validated for the case of particles subject to a one-dimensional (an-)harmonic and Morse potential using finite-differences for the advection part. Thereby, we verify the second order of convergence and observe non-classical behavior in the evolution of the Wigner function.

1. Introduction

The Wigner formalism, also known as quantum mechanics in phase space [1], provides an alternative but equivalent description of quantum mechanics in terms of a (quasi)-distribution function of the particle position and momentum. It has proven to provide a helpful supplement to operator methods in Hilbert space as well as to path integral formulations, and has offered new insights into the relation between quantum and classical physics, as it does not discriminate between coordinate and momentum space. For instance, it has been a fruitful perspective for the study of quantum chaos. In addition, it offers the opportunity to systematically consider quantum corrections to the classical dynamics by expanding the *quantum Liouville equation* around $\hbar \approx 0$. Nowadays, it is also a valuable tool in the fields of quantum optics as well as nuclear, plasma and semiconductor physics to describe transport processes, for example, in open quantum systems [1]. The Wigner function, introduced by E. Wigner in Ref. [2], is the Weyl transformation of the density matrix and a quasi-probability distribution that can "intuitively" account for scattering and decoherence effects in quantum systems [3,4]. It differs from a classical probability distributions as it can change sign during the evolution especially in regions where quantum interference effects become important. For a physical interpretation of negative values for the Wigner distribution, the interested reader should consult Ref. [5].

Since the Wigner equation was introduced in 1932, it has been tackled by various numerical approaches, such as finite differences [6,7], Fourier spectral collocation [8,9], deterministic particle [10,11], and Monte-Carlo [12,13], which can also handle the many-particle Wigner problem. Here, we extend the technique described in Refs. [8,9] to arbitrary basis functions $\phi_n(\vec{p})$ of $L^2(\mathbb{R}^d)$ in momentum-space and reveal the underlying mathematical structure of the resulting infinite-dimensional set of reaction–advection equations. By using this formulation we show that the action of the potential on the Wigner func-

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tion is a unitary rotation of its coefficient vector, whereas the advection operation can be discretized by various techniques used in computational fluid dynamics, such as finite difference, finite volume or finite element, cf. Ref. [14]. In that way, one is able to construct a finite element simulation of the Wigner evolution. Employing a more general basis we assume that the higher computational costs of our method, $\mathcal{O}(N^2)$, compared to $\mathcal{O}(N \log N)$ for the spectral Fourier decomposition are outweighed by a smaller number N of basis functions to obtain the same order of accuracy through focusing the computational effort to regions of interest, as for example in the case of Wigner functions that are strongly localized in momentum-space, such as particles in a periodic potential, cf. Bloch's theorem and Ref. [15]. In addition, the "artificial" periodization of the Wigner function can be avoided, which may mitigate the self-interaction of the distribution at the domain boundaries of the simulation that is present for the Fourier basis choice, cf. Ref. [16].

This article is organized as follows. First, we give an introduction to the Wigner formalism and present the properties of the Wigner equation, especially for the pseudo-differential operator. In section 3 we show the details of the numerical method to handle the obtained multi-dimensional reaction–advection equation. Thirdly, we validate the technique by simulating a one-dimensional (an-)harmonic oscillator, which offers the opportunity to compare with an analytical solution, cf. Ref. [17], such that we can perform a convergence analysis, and to observe quantum effects when the anharmonic potential is used. To study tunneling phenomena, we show the evolution of bounded states in the double well potential and measure the spread as well as the covariance of the Wigner function in phase space. In the last section, we will highlight the strengths and weaknesses of the approach.

2. Wigner formalism

Our aim is to simulate the time-evolution of the Wigner function $w(\tau, \vec{q}, \vec{p})$ of a d-dimensional system of non-relativistic spinless particles of mass m subject to the potential $U(\tau, \vec{q})$, based on the Wigner equation

$$0 = \partial_\tau w + \frac{\vec{p}}{m} \cdot \vec{\nabla}_q w + \Theta[U] w \,, \tag{1}$$

$$\Theta[U] \equiv \frac{\imath}{\hbar} \left[U(\tau, \vec{q} + \imath \hbar \vec{\nabla}_p / 2) - U(\tau, \vec{q} - \imath \hbar \vec{\nabla}_p / 2) \right] , \tag{2}$$

To understand the action of the operator $\Theta[U]$ one can use a Taylor expansion around $\hbar \approx 0$ to order N_a, to obtain an approximation of the Wigner equation to order $\mathcal{O}(\hbar^{N_a+1})$ if N_a is uneven or $\mathcal{O}(\hbar^{N_a+1})$ if N_a is even. Instead of the differential representation, one can also employ the integral form, which reads

$$\Theta[U] w = \frac{\imath}{\hbar} \int_{\mathbb{R}^d} \mathrm{d}\vec{\eta} \; \delta U(\tau, \vec{q}, \vec{\eta}) \tilde{w}(\tau, \vec{q}, \vec{\eta}) e^{-\imath \vec{\eta} \cdot \vec{p}} , \tag{3}$$

$$\delta U(\tau, \vec{q}, \vec{\eta}) \equiv U\left(\tau, \vec{q} + \frac{\hbar}{2}\vec{\eta}\right) - U\left(\tau, \vec{q} - \frac{\hbar}{2}\vec{\eta}\right) , \tag{4}$$

$$\tilde{w}(\tau, \vec{q}, \vec{\eta}) \equiv \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \mathrm{d}\vec{p}' \; w(\tau, \vec{q}, \vec{p}') e^{\imath \vec{\eta} \cdot \vec{p}'} \,. \tag{5}$$

The independent variables are time τ, space $\vec{q}$ and momentum $\vec{p}$ respectively. Hence, the Wigner function itself has the dimension h^{-d}, since it fulfills

$$\int_{\mathbb{R}^d} \mathrm{d}\vec{q} \int_{\mathbb{R}^d} \mathrm{d}\vec{p} \; w(\tau, \vec{q}, \vec{p}) = N_p \,, \tag{6}$$

where N_p is the number of particles in the system. To have an easier grasp on the equation, we make it dimensionless. First of all, we measure the Wigner function with respect to $\hbar^d$, i.e. we introduce the dimensionless Wigner function $W(\tau, \vec{q}, \vec{p}) \equiv \hbar^d w(\tau, \vec{q}, \vec{p}) / N_p$, and we employ the following scaling relations

$$\vec{x} = \vec{q}/l \,, t = \tau/T \,, \vec{v} = \frac{T}{lm}\vec{p} \,, V(t, \vec{x}) = U(\tau, \vec{q})/\bar{U} \,, \tag{7}$$

described in Ref. [18]. Thus, we obtain the dimensionless Wigner equation

$$0 = \partial_t W + \vec{v} \cdot \vec{\nabla}_x W + \Theta[V] W \,, \tag{8}$$

$$\Theta[V] \equiv \frac{\imath B}{\epsilon} \left[V\left(t, \vec{x} + \frac{\imath\epsilon}{2}\vec{\nabla}_v\right) - V\left(t, \vec{x} - \frac{\imath\epsilon}{2}\vec{\nabla}_v\right) \right] , \tag{9}$$

where we have introduced the dimensionless constants

$$\epsilon \equiv \frac{\hbar T}{l^2 m} \,, B \equiv \frac{\bar{U} T^2}{l^2 m} \,, \tag{10}$$