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A Branching Random Walk Method for Many-Body Wigner Quantum Dynamics

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Abstract. A branching random walk algorithm for many-body Wigner equations and its numerical applications for quantum dynamics in phase space are proposed and analyzed in this paper. Using an auxiliary function, the truncated Wigner equation and its adjoint form are cast into integral formulations, which can be then reformulated into renewal-type equations with probabilistic interpretations. We prove that the first moment of a branching random walk is the solution for the adjoint equation. With the help of the additional degree of freedom offered by the auxiliary function, we are able to produce a weighted-particle implementation of the branching random walk. In contrast to existing signed-particle implementations, this weighted-particle one shows a key capacity of variance reduction by increasing the constant auxiliary function and has no time discretization errors. Several canonical numerical experiments on the 2D Gaussian barrier scattering and a 4D Helium-like system validate our theoretical findings, and demonstrate the accuracy, the efficiency, and thus the computability of the proposed weighted-particle Wigner branching random walk algorithm.

AMS subject classifications: 60J85, 81S30, 45K05, 65M75, 82C10, 81V70, 81Q05

Key words: Wigner equation, branching random walk, quantum dynamics, variance reduction, signed-particle Monte Carlo method, adjoint equation, renewal-type equations, importance sampling, resampling.

1. Introduction

Connection between partial differential equations (PDE) and stochastic processes is an active topic in modern mathematics and provides powerful tools for both probability theory and analysis, especially for PDE of elliptic and parabolic type [1, 2]. In the past few decades, their numerical applications have also burgeoned with a lot of developments, such as the ensemble Monte Carlo method for the Boltzmann transport equation [3–6], the random walk method for the Laplace equation [7] and the diffusion Monte Carlo method for the Schrödinger equation [8,9]. In particular, the diffusion Monte Carlo method allows

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us to go beyond the mean-field approximation and offer a reliable ground state solution to quantum many-body systems. In this work, we focus on the probabilistic approach to the equivalent phase space formalism of quantum mechanics, namely, the Wigner function approach [10], which bears a close analogy to classical mechanics. In recent years, the Wigner equation has been drawing growing attention [11–14] and widely used in nano-electronics [15,16], non-equilibrium statistical mechanics [17], quantum optics [18], and many-body quantum systems [19]. Actually, a branch of experiment physics in the community of quantum tomography is devoting to reconstructing the Wigner function from measurements [20,21]. Moreover, the intriguing mathematical structure of the Weyl-Wigner correspondence has also been employed in the deformation quantization [22].

In contrast to its great theoretical advantages, the Wigner equation is extremely difficult to be solved because of the high dimensionality of the phase space as well as the highly oscillating structure of the Wigner function due to the spatial coherence [12,21]. Although several efficient deterministic solvers, e.g., the conservative spectral element method (SEM) [23] and the third-order advective-spectral-mixed scheme (ASM) [24], have enabled an accurate transient simulation in 2D and 4D phase space, they are still limited by data storage and increasing computational complexity. One possible approach to solving the higher dimensional problems is the Wigner Monte Carlo method, which displays $N^{-\frac{1}{2}}$ convergence (N is the number of samples), regardless of the dimensionality, and scales much better on parallel computing platforms [19,25].

This work is motivated by a recently developed stochastic method, termed the signed-particle Wigner Monte Carlo method (spWMC) [26–28]. *A particle carrying a signed weight, either* -1 *or* $+1$*, is called a signed particle.* This method utilizes the branching of signed particles to capture the quantum coherence, and the numerical accuracy has been validated in 2D situations [29–31]. Very recently, it has been also validated theoretically by exploiting the connection between a piecewise-deterministic Markov process and the weak formulation of the Wigner equation and a random cloud (RC) method was presented [32][1]. In this work, we use an alternative approach to constructing the mathematical framework for spWMC from the viewpoint of computational mathematics, namely, we focus on the probabilistic interpretation of the mild solution of the (truncated) Wigner equation and its adjoint correspondence. In particular, we would like to point out that the resulting stochastic model, the importance sampling and the resampling are three components of a computable scheme for simulating the many-body Wigner quantum dynamics.

Our first objective is to explore the inherent relation between the Wigner equation and a stochastic branching random walk model, as sketched by the diagram below.

$$\boxed{\text{Wigner equation}} \xrightarrow[\gamma(\boldsymbol{x})]{\text{integral form}} \boxed{\text{Renewal-type equation}} \xleftarrow{\text{moment}} \boxed{\text{Branching random walk}} \tag{1.1}$$

With an auxiliary function $\gamma(\boldsymbol{x})$, we can cast the Wigner equation (as well as its adjoint equation) into a renewal-type integral equation and prove that its solution is equivalent to

[1]We started this work and finished the first version of the manuscript [33] without being aware of the research in [32]. As a consequence, we adopt different mathematical treatments for the Wigner equation and thus propose a different stochastic algorithm the variance of which can be systematically reduced.