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The Wigner Branching Random Walk: Efficient Implementation and Performance Evaluation

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Abstract. To implement the Wigner branching random walk, the particle carrying a signed weight, either -1 or $+1$, is more friendly to data storage and arithmetic manipulations than that taking a real-valued weight continuously from -1 to $+1$. The former is called a signed particle and the latter a weighted particle. In this paper, we propose two efficient strategies to realize the signed-particle implementation. One is to interpret the multiplicative functional as the probability to generate pairs of particles instead of the incremental weight, and the other is to utilize a bootstrap filter to adjust the skewness of particle weights. Performance evaluations on the Gaussian barrier scattering (2D) and a Helium-like system (4D) demonstrate the feasibility of both strategies and the variance reduction property of the second approach. We provide an improvement of the first signed-particle implementation that partially alleviates the restriction on the time step and perform a thorough theoretical and numerical comparison among all the existing signed-particle implementations. Details on implementing the importance sampling according to the quasi-probability density and an efficient resampling or particle reduction are also provided.

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Key words: Wigner equation, branching random walk, signed particle, bootstrapping, weighted particle, Monte Carlo method, quantum dynamics, importance sampling, resampling, particle reduction.

1 Introduction

The Wigner function $f(\boldsymbol{x},\boldsymbol{k},t)$ for a N-body d-dimensional quantum system lives in the phase space $(\boldsymbol{x},\boldsymbol{k})\in\mathbb{R}^{2n}$ with $n=Nd$ for position $\boldsymbol{x}$ and wavevector $\boldsymbol{k}$, and satisfies the following Wigner equation (WEQ) [1]

$$\frac{\partial}{\partial t}f(\boldsymbol{x},\boldsymbol{k},t)+\frac{\hbar\boldsymbol{k}}{\boldsymbol{m}}\cdot\nabla_x f(\boldsymbol{x},\boldsymbol{k},t)=\Theta_V[f](\boldsymbol{x},\boldsymbol{k},t), \tag{1.1}$$

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where the pseudo-differential operator is characterized by a convolution with the Wigner kernel V_W

$$\Theta_V[f](\boldsymbol{x},\boldsymbol{k},t)=\int_{\mathbb{R}^n}\mathrm{d}\boldsymbol{k}'V_W(\boldsymbol{x},\boldsymbol{k}-\boldsymbol{k}',t)f(\boldsymbol{x},\boldsymbol{k}',t), \tag{1.2}$$

$$V_W(\boldsymbol{x},\boldsymbol{k},t)=\frac{1}{\mathbb{i}\hbar(2\pi)^n}\int_{\mathbb{R}^n}\mathrm{d}\boldsymbol{y}\mathbb{e}^{-\mathbb{i}\boldsymbol{k}\cdot\boldsymbol{y}}\left[V\left(\boldsymbol{x}+\frac{\boldsymbol{y}}{2},t\right)-V\left(\boldsymbol{x}-\frac{\boldsymbol{y}}{2},t\right)\right], \tag{1.3}$$

provided that $V(\boldsymbol{x},t)$ belongs to an appropriate symbol class, $\hbar$ is the reduced Planck constant, $\boldsymbol{k}/\boldsymbol{m}$ is short for $(\boldsymbol{k}_1/m_1,\cdots,\boldsymbol{k}_N/m_N)$ and m_i is the mass of the i-th body. In the past few decades, WEQ has been drawing a growing attention, especially in the simulations of nanodevices [2–7] as well as the many-body quantum mechanics [8,9], due to its theoretical advantage [10,11].

The huge challenge to numerical resolution of WEQ lies in the high dimensionality of phase space, which is unfriendly to traditional deterministic solvers. By contrast, stochastic methods may provide a promising approach to overcoming the curse of dimensionality, and several attempts have also revealed its feasibility in capturing fine structures of 2D and 4D quantum systems [9,12–14]. The most remarkable feature there is the pair generation of particles (or branching of particle in probabilistic terminology), which intends to control the variance and ameliorate the "negative sign problem" [15–17]. It has recently been shown that the corresponding rigorous mathematical theory consists of three components: the probabilistic interpretation of WEQ, the principle of importance sampling and the technique of density estimation [9,18].

Although almost all Monte Carlo approaches rely on the equivalent stochastic interpretation of WEQ, there exist significant differences between various realizations and thereby resulting in distinct performances. Thus it screams for fair and detailed evaluations to demonstrate how numerical accuracy is influenced by several elements, including the way to truncate the WEQ, the choice of the auxiliary function $\gamma(\boldsymbol{x})$ that characterizes the life-length of particles and the interpretation of the multiplicative functionals. The first signed particle Wigner Monte Carlo method (abbreviated as **sp0**) is suggested to choose a variable auxiliary function $\gamma(\boldsymbol{x})$ and confine the particle weights to either $+1$ or -1 (termed the signed particle) [17,19]. Such setting greatly facilitates the data storage and the arithmetic operation, but poses a limitation on the time step in order to maintain the accuracy. In this work, we will propose an improvement (**I**) to alleviate such limitation via a proper treatment of the bias term and denote the resulting scheme by **sp0-I**. Another class of stochastic algorithms based on the random cloud model (abbreviated as **RC**) has been proposed in [13,18], where a constant time technique and a rejection sampling technique are adopted for generating the scattering time and state, respectively [20]. In our previous work, we have proposed the Wigner branching random walk (WBRW) model, in which the multiplicative functionals are interpreted as the importance weights, yielding the weighted-particle branching random walk algorithm (abbreviated as **wp**) [9]. Simulating the WBRW ameliorates the restriction on the time step and allows a reduction in variance by choosing a large constant $\gamma(\boldsymbol{x})$. The price to