

BRANCHING RANDOM WALK SOLUTIONS TO THE WIGNER EQUATION*

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Abstract. We analyze the stochastic solutions to the Wigner equation, which explain the nonlocal oscillatory integral operator Θ_V with an antisymmetric kernel as the generator of two branches of jump processes. All existing branching random walk solutions are formulated based on the Hahn–Jordan decomposition $\Theta_V = \Theta_V^+ - \Theta_V^-$, i.e., treating Θ_V as the difference of two positive operators Θ_V^\pm , each of which characterizes the transition of states for one branch of particles. Despite the fact that the first moments of such models solve the Wigner equation, we prove that the bounds of corresponding variances grow exponentially in time, with the rate depending on the upper bound of Θ_V^\pm instead of Θ_V . In other words, the decay of high-frequency components is totally ignored, resulting in a severe numerical sign problem. To fully utilize such a decay property, we turn to the stationary phase approximation for Θ_V , which captures essential contributions from the stationary phase points as well as from the near-cancellation of positive and negative weights. The resulting branching random walk solutions are then proved to asymptotically solve the Wigner equation, but they gain a substantial reduction in variances, thereby ameliorating the sign problem. Numerical experiments in 4-D phase space validate our theoretical findings.

Key words. Wigner equation, branching random walk, stationary phase approximation, non-local operator, sign problem, variance reduction

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1. Introduction. We discuss the probabilistic interpretation of the Wigner equation defined in phase space $(\mathbf{x}, \mathbf{k}) \in \mathbb{R}^n \times \mathbb{R}^n$ [1, 2, 3], arising from recent stochastic methods for simulating the Wigner dynamics in semiconductors, quantum devices, and many-body quantum systems [4, 5, 6, 7, 8, 9, 10]. Our starting point is the (adjoint) integral form of the Wigner equation with an “initial” condition $\varphi_T \in L^2(\mathbb{R}^n \times \mathbb{R}^n)$,

$$(1.1) \quad \begin{aligned} \varphi(\mathbf{x}, \mathbf{k}, t) = & (1 - \mathcal{G}(T-t))\varphi_T(\mathbf{x}(T-t), \mathbf{k}) \\ & - \int_t^T d\mathcal{G}(t'-t) \left\{ \frac{\Theta_V[\varphi](\mathbf{x}(t'-t), \mathbf{k}', t')}{\gamma_0} - \varphi(\mathbf{x}(t'-t), \mathbf{k}, t') \right\}, \end{aligned}$$

where $\varphi(\mathbf{x}, \mathbf{k}, t)$ is the dual Wigner function, $\mathbf{x}(\Delta t) = \mathbf{x} + \frac{\hbar \mathbf{k}}{m} \Delta t$ is the forward-in-time trajectory of (\mathbf{x}, \mathbf{k}) with a positive time increment Δt , m is the mass, \hbar is the reduced Planck constant, and $\mathcal{G}(t) = 1 - e^{-\gamma_0 t}$ is an exponential distribution with a constant intensity γ_0 [10]. Here the pseudodifferential operator (Ψ DO) Θ_V reads as

$$(1.2) \quad \Theta_V[\varphi](\mathbf{x}, \mathbf{k}, t) = \frac{1}{i\hbar(2\pi)^n} \iint_{\mathbb{R}^n \times \mathbb{R}^n} e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{y}} D_V(\mathbf{x}, \mathbf{y}, t) \varphi(\mathbf{x}, \mathbf{k}', t) d\mathbf{y} d\mathbf{k}',$$

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where the symbol function $D_V(\mathbf{x}, \mathbf{y}, t) = V(\mathbf{x} - \mathbf{y}/2, t) - V(\mathbf{x} + \mathbf{y}/2, t)$ is the central difference of the potential $V(\mathbf{x}, t)$.

The reader can refer to a vast number of articles; see, e.g., [2, 11, 5, 10] for the detailed derivation of (1.1).

It is well known that Θ_V , a nonlocal operator with an antisymmetric symbol, i.e., $D_V(\mathbf{x}, \mathbf{y}, t) = -D_V(\mathbf{x}, -\mathbf{y}, t)$, characterizes a deformation of the classical Poisson bracket [12] and exactly reflects the nonlocal nature of quantum mechanics [13, 14, 15, 16]. Two equivalent representations of Ψ DO will be investigated in subsequent analysis. One is the kernel representation,

$$(1.3) \quad \Theta_V[\varphi](\mathbf{x}, \mathbf{k}, t) = \int_{\mathbb{R}^n} V_W(\mathbf{x}, \mathbf{k} - \mathbf{k}', t) \varphi(\mathbf{x}, \mathbf{k}', t) d\mathbf{k}',$$

with the real-valued kernel function V_W (termed the Wigner kernel),

$$(1.4) \quad V_W(\mathbf{x}, \mathbf{k}, t) = \frac{1}{i\hbar(2\pi)^n} \int_{\mathbb{R}^n} \left(V\left(\mathbf{x} - \frac{\mathbf{y}}{2}, t\right) - V\left(\mathbf{x} + \frac{\mathbf{y}}{2}, t\right) \right) e^{i\mathbf{k}\cdot\mathbf{y}} dy.$$

The other is the oscillatory integral representation,

$$(1.5) \quad \Theta_V[\varphi](\mathbf{x}, \mathbf{k}, t) = \int_{\mathbb{R}^n} e^{iz(\mathbf{x})\cdot\mathbf{k}'} \psi(\mathbf{k}', t) \left(\varphi\left(\mathbf{x}, \mathbf{k} - \frac{\mathbf{k}'}{2}, t\right) - \varphi\left(\mathbf{x}, \mathbf{k} + \frac{\mathbf{k}'}{2}, t\right) \right) d\mathbf{k}',$$

where $\psi(\mathbf{k}, t)$ denotes the amplitude function,

$$(1.6) \quad \psi(\mathbf{k}, t) = \frac{1}{i\hbar(2\pi)^n} e^{-i\mathbf{k}\cdot z(\mathbf{x})} \int_{\mathbb{R}^n} V(\mathbf{x}, t) e^{-i\mathbf{k}\cdot\mathbf{x}} dx.$$

For an example of a quantum system composed of a two-body interaction $V(\mathbf{x}) = V(|\mathbf{x} - \mathbf{x}_A|)$ with \mathbf{x}_A a fixed position, the oscillatory integral representation (1.5) is more relevant because $z(\mathbf{x}) = \mathbf{x} - \mathbf{x}_A$ directly presents the spatial displacement between two bodies [2]. A key observation is that the oscillatory integral operator decays as the integrand becomes more and more oscillated. In fact, as stated by Hörmander's theorem [17], if the amplitude function ψ is sufficiently smooth and compactly supported, then it has a sharp estimate for sufficiently large $|z(\mathbf{x})|$,

$$(1.7) \quad \|\Theta_V[\varphi](\mathbf{x}, \mathbf{k}, t)\|_{L_k^2} \leq C|z(\mathbf{x})|^{-n/2} \|\varphi(t)\|_{L_k^2},$$

which reflects the transparent fact that the nonlocal quantum interaction decays as the two-body distance increases. For instance, the decay rate of the Morse potential in section 5 is $\mathcal{O}(|z(\mathbf{x})|^{-1})$ in contrast to the exponential decay rate of its classical counterpart.

Stochastic interpretation of the Wigner equation is motivated by its close analogue, the classical particle transport [4, 11, 18, 19] and scattering interpretation of Ψ DO [2, 5]. Intuitively speaking, the formal Neumann series expansion of (1.1) can be interpreted as the expectation of stochastic trajectories over Poisson jumps. The major problem is how to resolve the negative values of V_W . Unlike nonlocal operators with nonnegative and symmetric kernels which have apparent probabilistic meanings [20, 21, 22], all existing stochastic interpretations of the Wigner kernel are based on the decomposition of the antisymmetric kernel [4, 8, 9, 10]

$$(1.8) \quad V_W(\mathbf{x}, \mathbf{k}, t) = V_W^+(\mathbf{x}, \mathbf{k}, t) - V_W^-(\mathbf{x}, \mathbf{k}, t), \quad V_W^\pm(\mathbf{x}, \mathbf{k}, t) = \max\{\pm V_W(\mathbf{x}, \mathbf{k}, t), 0\},$$

which, in turn, gives rise to the unique Hahn–Jordan decomposition (HJD),

$$(1.9) \quad \Theta_V[\varphi] = \Theta_V^+[\varphi] - \Theta_V^-[\varphi], \quad \Theta_V^\pm[\varphi](\mathbf{x}, \mathbf{k}, t) = \int_{\mathbb{R}^n} V_W^\pm(\mathbf{x}, \mathbf{k} - \mathbf{k}', t) \varphi(\mathbf{x}, \mathbf{k}', t) d\mathbf{k}'.$$

If $V_W^\pm \in C([0, T], L_{loc}^1(\mathbb{R}^n \times \mathbb{R}^n))$ with a normalizing function $\xi(\mathbf{x}, t)$ in a finite \mathbf{k} -domain, $V_W^\pm(\mathbf{x}, \mathbf{k}, t)/\xi(\mathbf{x}, t)$ become probability densities and characterize the transitions in \mathbf{k} -space, and $\xi(\mathbf{x}, t)/\gamma_0$, $-\xi(\mathbf{x}, t)/\gamma_0$, and 1 are regarded as importance weights for three branches of new particles, respectively. In probability theory, such a stochastic model that exhibits both random motion and particle growth is called the branching random walk (BRW), since it describes the random walk of particles reproducing according to the Galton–Watson process [19, 23]. Another pivotal issue is interpretation of particle weights. Under different settings of $\xi(\mathbf{x}, t)/\gamma_0$, stochastic models can be divided into two categories. The first is the signed-particle version including the signed-particle Wigner Monte Carlo [5, 6, 7] and random cloud algorithms [9], where particle weights are confined in a two-valued set $\{-1, 1\}$. Both algorithms can be recovered by the signed-particle Wigner branching random walk (WBRW) model if we are replacing the constant intensity γ_0 with $\xi(\mathbf{x}, t)$ or interpreting $\xi(\mathbf{x}, t)/\gamma_0$ as the probability to generate particles. The second category is the weighted-particle WBRW, where particles take weights from a continuous domain $[-1, 1]$. In particular, numerical simulations show that variance of the latter can be systematically reduced by increasing γ_0 to boost the generation of particles, whereas both variance and particle growth rate of the former are not influenced by γ_0 [24].

Despite pictorial descriptions with physical intuitions, rigorous analysis of stochastic Wigner algorithms is rarely found except for that based on asymptotics [5, 6]. It was not until very recently that the connection between solutions of (1.1) and first moments of stochastic models was well established in probabilistic languages [8, 10]. However, to the best of our knowledge, it still lacks a theoretical investigation of variances, even though they are of significant importance for analyzing the properties of stochastic algorithms. To this end, the first contribution of this work is concentrated on estimating the second moments of WBRW under HJD (dubbed WBRW-HJD hereafter). We prove that its variances grow exponentially in time with the exponential rates $2\xi^2/\gamma_0$ for the weighted-particle version and 2ξ for the signed-particle counterpart, where ξ gives a uniform upper bound of $\xi(\mathbf{x}, t)$. In other words, it explains why the weighted-particle implementation helps ameliorate the numerical sign problem, a fundamental bottleneck in quantum Monte Carlo simulations [25, 26].

Our second contribution is formulating a new class of BRW solutions to asymptotically solve the Wigner equation and gain a significant reduction in variances. According to our resulting theoretical bounds, we point out that the rapid growth of variances is rooted in the splitting of the Wigner kernel because it totally ignores the decay property of Ψ DO as stated in (1.7). In order to fully seize such decay, we adopt the stationary phase approximation (SPA) [27] to the high-frequency component of Ψ DO, which captures the essential contribution from two radial integrals. As a consequence, WBRW under SPA (dubbed WBRW-SPA hereafter) alleviates the numerical sign problem, especially in the region where $|\mathbf{z}(\mathbf{x})|$ is sufficiently large, which is crucial for accurate high-dimensional Wigner simulations.

The rest of the paper is organized as follows. Section 2 states our main results. The variances of WBRW-HJD are analyzed in section 3. Section 4 gives an estimate of asymptotic errors in SPA to Ψ DO and analyzes the properties of WBRW-SPA. In section 5, a typical numerical experiment is performed to verify our theoretical

findings. The conclusion and a discussion are drawn in section 6.

2. Statement of main results. Before proceeding to the three main theorems of this work, several definitions and notation are introduced in this section.

2.1. Definitions and notation. Suppose $\varphi(\mathbf{x}, \mathbf{k}, t)$ has a compact support $\mathcal{X} \times \mathcal{K}$ in phase space \mathbb{R}^{2n} over a finite time interval $[0, T]$ and that $V_W^\pm \in C([0, T], L^1_{loc}(\mathbb{R}^n \times \mathbb{R}^n))$; then for $R = 2|\mathcal{K}|$ with $|\mathcal{K}|$ the diagonal length of \mathcal{K} , there exist a normalizing function $\xi(\mathbf{x}, t)$ and a uniform upper bound $\check{\xi}$,

$$(2.1) \quad \xi(\mathbf{x}, t) = \int_{\mathbb{R}^n} V_W^\pm(\mathbf{x}, \mathbf{k}, t) \mathbb{1}_{B(R)}(\mathbf{k}) d\mathbf{k}, \quad \check{\xi} = \max_{0 \leq t \leq T} \max_{\mathbf{x} \in \mathcal{X}} \xi(\mathbf{x}, t),$$

where $B(r)$ is a closed ball with radius r centered at the origin, and $\mathbb{1}_S(\cdot)$ is the characteristic function on a set S . The constant intensity γ_0 satisfies $\gamma_0 \geq \check{\xi}$. Under appropriate assumptions on $\psi(\mathbf{k}, t)$ in (1.6) (see (A3) in section 2.2), we can choose a radial function $\Psi(|\mathbf{k}|) \in L^1_{loc}(\mathbb{R}^n)$, such that $|\psi(\mathbf{k}, t)| \leq \Psi(|\mathbf{k}|)$ in $\mathbb{R}^n \setminus \{0\}$ and $\check{\eta} = \int_0^\infty r^{n-1} \Psi(r) \mathbb{1}_{[0, R]}(r) dr < \infty$.

For SPA, a frequency decomposition of PDO with a fixed filter λ_0 is adopted, and the low-frequency component reads as

$$\Lambda^{\leq \lambda_0}[\varphi](\mathbf{x}, \mathbf{k}, t) = \int_{B(\lambda_0/|\mathbf{z}(\mathbf{x})|)} e^{i\mathbf{z}(\mathbf{x}) \cdot \mathbf{k}'} \psi(\mathbf{k}', t) \Delta_{\mathbf{k}'}[\varphi](\mathbf{x}, \mathbf{k}, t) d\mathbf{k}',$$

with the central difference operator $\Delta_{\mathbf{k}'}[\varphi](\mathbf{x}, \mathbf{k}, t) = \varphi(\mathbf{x}, \mathbf{k} - \frac{\mathbf{k}'}{2}, t) - \varphi(\mathbf{x}, \mathbf{k} + \frac{\mathbf{k}'}{2}, t)$. After applying SPA, we have two principal terms of asymptotic expansion of the high-frequency component $\Lambda^{>\lambda_0} := \Theta_V[\varphi] - \Lambda^{\leq \lambda_0}[\varphi]$,

$$\Lambda_\pm^{>\lambda_0}[\varphi](\mathbf{x}, \mathbf{k}, t) = \int_{\frac{\lambda_0}{|\mathbf{z}(\mathbf{x})|}}^{+\infty} e^{\pm i r |\mathbf{z}(\mathbf{x})|} \left(\frac{2\pi}{\pm i r |\mathbf{z}(\mathbf{x})|} \right)^{\frac{n-1}{2}} r^{n-1} \psi(r \sigma_\pm, t) \Delta_{r \sigma_\pm}[\varphi](\mathbf{x}, \mathbf{k}, t) dr,$$

where σ_\pm (short for $\sigma_\pm(\mathbf{x})$) represent two critical points on the $(n-1)$ -D unit spherical surface with normal vectors pointing in (or opposite to) the direction of $\mathbf{z}(\mathbf{x}) = (z_1, z_2, \dots, z_n)$ and can be parameterized by

$$\sigma_\pm = (\cos \vartheta_1^\pm, \sin \vartheta_1^\pm \cos \vartheta_2^\pm, \dots, \sin \vartheta_1^\pm \cdots \sin \vartheta_{n-2}^\pm \cos \vartheta_{n-1}^\pm, \sin \vartheta_1^\pm \cdots \sin \vartheta_{n-1}^\pm),$$

with

$$(2.2) \quad \begin{aligned} \vartheta_i^\pm &= \arccot(\pm z_i / \sqrt{z_{i+1}^2 + \cdots + z_n^2}) \in [0, \pi], \quad i = 1, 2, \dots, n-2, \\ \vartheta_{n-1}^\pm &= 2 \arccot(\pm (\sqrt{z_{n-1}^2 + z_n^2} + z_{n-1}) / z_n) \in [0, 2\pi]. \end{aligned}$$

Hence, the real-valued SPA to PDO $\Theta_V[\varphi]$, denoted by $\Theta_V^{\lambda_0}[\varphi]$, can be collected as

$$(2.3) \quad \Theta_V^{\lambda_0}[\varphi](\mathbf{x}, \mathbf{k}, t) = \Lambda^{\leq \lambda_0}[\varphi](\mathbf{x}, \mathbf{k}, t) + \Lambda_+^{>\lambda_0}[\varphi](\mathbf{x}, \mathbf{k}, t) + \Lambda_-^{>\lambda_0}[\varphi](\mathbf{x}, \mathbf{k}, t),$$

which makes no change on $\Lambda^{\leq \lambda_0}$ containing relevant nonlocal quantum effects and captures the major contribution of $\Lambda^{>\lambda_0}$ by two branches of radial integrals.

Remark 1. One should note that SPA is essentially different from the semiclassical treatment in [28]. The latter suggests excluding the high-frequency component $\Lambda^{>\lambda_0}$ of PDO directly and replacing the low-frequency $\Lambda^{\leq \lambda_0}$ by a nonlocal “classical” force,

based on a linearization of φ : $\varphi(\mathbf{x}, \mathbf{k} - \mathbf{k}', t) \approx -\mathbf{k}' \cdot \nabla_{\mathbf{k}} \varphi(\mathbf{x}, \mathbf{k}, t)$. In principle, one can seek a combination of both approaches by further splitting $\Lambda^{\leq \lambda_0}$ in (2.3) into a low-frequency term and a mid-frequency one, so that the linearization of φ may seize the localization of the former integral over very small wave numbers.

Since the probabilistic space $(\Omega, \mathcal{F}, \Pi_Q)$ of WBRW is well delineated in [10], we just mention it briefly for the sake of descriptive integrality. The random variable in WBRW is the family history [23, 29] standing for a random sequence $\omega = \{(\tau_0, Q_0, w_0); (\tau_1, Q_1, w_1); (\tau_{11}, Q_{11}, w_{11}); \dots\}$, where $Q_i = (\mathbf{x}_i, \mathbf{k}_i)$ appears in a definite order of enumeration; $\tau_i, \mathbf{x}_i, \mathbf{k}_i, w_i$ denote the life-length, starting position, wavevector, and particle weight of the i th particle, respectively. Ω collects all family histories.

The motion of each particle, starting at instant t and state (\mathbf{x}, \mathbf{k}) and carrying a weight w , is described by a right continuous Markov process and dies in the age time interval $(t, t + \tau)$ with probability $1 - e^{-\gamma_0 \tau}$. It is either frozen at state $(\mathbf{x}(T - t), \mathbf{k})$ when its life-length $\tau \geq T - t$, or killed at instant $t + \tau$ and produces at most five mutually independent offspring at states $(\mathbf{x}_{(1)}, \mathbf{k}_{(1)}), (\mathbf{x}_{(2)}, \mathbf{k}_{(2)}) \dots (\mathbf{x}_{(5)}, \mathbf{k}_{(5)})$, endowed with updated weights $w_{(1)}, w_{(2)}, \dots, w_{(5)}$, respectively.

Suppose $(\mathbf{x}_i, \mathbf{k}_i)$ is the starting state of a frozen particle i in a given family history ω , and the collection of frozen particles starting at t is denoted by $\mathcal{E}_t(\omega)$. Then the WBRW model is given by

$$(2.4) \quad X_t(\omega) = \sum_{i \in \mathcal{E}_t(\omega)} \hat{w}_i \cdot \varphi_T(\mathbf{x}_i(T - t_i), \mathbf{k}_i),$$

where the cumulative weight \hat{w}_i for $i = \langle i_1 i_2 \dots i_n \rangle$ is the product of the particle weights $w_{i_1 \dots i_m} \in [-1, 1]$: $\hat{w}_i = \prod_{m=1}^n (-1)^{i_m+1} w_{i_1 \dots i_m} \in [-1, 1]$.

For WBRW-HJD, the random jumps $\mathbf{k}_{i_1 \dots i_m} - \mathbf{k}_{i_1 \dots i_{m-1}}$ for $i_m = 1, 2$ are characterized by the transition density $V_W^\mp(\mathbf{x}, \mathbf{k}, t)/\xi(\mathbf{x}, t)$, respectively, while for WBRW-SPA, the random increments $r_{i_1 \dots i_m} = 2 |\mathbf{k}_{i_1 \dots i_m} - \mathbf{k}_{i_1 \dots i_{m-1}}|$ obey the transition density $r^{n-1} \Psi(r)/\check{\eta}$ in radial coordinate instead.

Let the initial particle weight $w_0 = 1$, and adopt the shorthand notation $\mathbf{z}_{i_1 \dots i_m} = \mathbf{z}(\mathbf{x}_{i_1 \dots i_m})$ and $\zeta_{i_1 \dots i_m} = \zeta(r_{i_1 \dots i_m}, \mathbf{x}_{i_1 \dots i_m}, t_{i_1 \dots i_m})$, where

$$\begin{aligned} \zeta(r, \mathbf{x}, t) &= e^{ir|\mathbf{z}(\mathbf{x})|} \left(\frac{2\pi}{ir|\mathbf{z}(\mathbf{x})|} \right)^{\frac{n-1}{2}} \frac{\psi(r\sigma_+, t)}{\Psi(r)}, \\ \sigma_{i_1 \dots i_m} &= \begin{cases} \frac{\xi(\mathbf{x}_{i_1 \dots i_m}, t_{i_1 \dots i_m})}{\gamma_0} \cdot \mathbb{1}_{[0, 2\lambda_0/|\mathbf{z}_{i_1 \dots i_m}|]}(r_{i_1 \dots i_m}), & i_m = 1, 2, \\ \frac{2\check{\eta}}{\gamma_0} \cdot |\text{Im}[\zeta_{i_1 \dots i_m}]| \cdot \mathbb{1}_{(\lambda_0/|\mathbf{z}_{i_1 \dots i_m}|, +\infty)}(r_{i_1 \dots i_m}), & i_m = 3, 4. \end{cases} \end{aligned}$$

Then the particle weight $w_{i_1 \dots i_m}$ can be specified below within different models.

(1) For the weighted-particle WBRW-HJD,

$$(2.5) \quad w_{i_1 \dots i_m} = \begin{cases} \frac{\xi(\mathbf{x}_{i_1 \dots i_m}, t_{i_1 \dots i_m})}{\gamma_0} \cdot \mathbb{1}_{\mathcal{K}}(\mathbf{k}_{i_1 \dots i_m}), & i_m = 1, 2, \\ 1, & i_m = 3. \end{cases}$$

(2) For the signed-particle WBRW-HJD, for $i_m \leq 2$,

$$(2.6) \quad w_{i_1 \dots i_m} = \begin{cases} 1 & \text{with } \Pr = \frac{\xi(\mathbf{x}_{i_1 \dots i_m}, t_{i_1 \dots i_m})}{\gamma_0} \cdot \mathbb{1}_{\mathcal{K}}(\mathbf{k}_{i_1 \dots i_m}), \\ 0 & \text{otherwise,} \end{cases}$$

and $w_{i_1 \dots i_m} = 1$ for $i_m = 3$.

(3) For the weighted-particle WBRW-SPA,

$$(2.7) \quad w_{i_1 \dots i_m} = \begin{cases} \sigma_{i_1 \dots i_m} \cdot \mathbb{1}_{\mathcal{K}}(\mathbf{k}_{i_1 \dots i_m}), & i_m = 1, 2, \\ \sigma_{i_1 \dots i_m} \cdot \text{sgn}(\text{Im}[\zeta_{i_1 \dots i_m}]) \cdot \mathbb{1}_{\mathcal{K}}(\mathbf{k}_{i_1 \dots i_m}), & i_m = 3, 4, \\ 1, & i_m = 5. \end{cases}$$

(4) For the signed-particle WBRW-SPA, for $i_m \leq 4$,

$$(2.8) \quad w_{i_1 \dots i_m} = \begin{cases} 1 & \text{with } \Pr = \sigma_{i_1 \dots i_m} \cdot \mathbb{1}_{\mathcal{K}}(\mathbf{k}_{i_1 \dots i_m}), \quad i_m = 1, 2, \\ \text{sgn}(\text{Im}[\zeta_{i_1 \dots i_m}]) & \text{with } \Pr = \sigma_{i_1 \dots i_m} \cdot \mathbb{1}_{\mathcal{K}}(\mathbf{k}_{i_1 \dots i_m}), \quad i_m = 3, 4, \\ 0 & \text{otherwise,} \end{cases}$$

and $w_{i_1 \dots i_m} = 1$ for $i_m = 5$.

Here $\text{sgn}(x) = 1$ for $x > 0$, $\text{sgn}(x) = -1$ for $x < 0$, and $\text{sgn}(x) = 0$ for $x = 0$.

2.2. Main results. In order to extend Ψ DO Θ_V to a bounded operator from $L^2(\mathbb{R}^{2n})$ to itself, e.g., there exists a uniform upper bound K_V such that

$$(2.9) \quad \|\Theta_V[\varphi](t)\|_2 \leq K_V \|\varphi(t)\|_2,$$

we make the following assumptions for a finite time interval $[0, T]$, where $\|\cdot\|_p$ is short for the $L_x^p \times L_{\mathbf{k}}^p$ norm. The L^2 -boundedness of Θ_V is readily verified by Young's convolution inequality or the Hardy–Littlewood–Sobolev theorem.

- (A1) $\varphi \in C([0, T], L^2(\mathbb{R}^n \times \mathbb{R}^n))$ and is localized in (\mathbf{x}, \mathbf{k}) -space for any $t \in [0, T]$, with the *minimal* compact support denoted by $\mathcal{X} \times \mathcal{K} \subset \mathbb{R}^n \times \mathbb{R}^n$.
- (A2) Either of the following conditions holds:
 - (1) $\psi \in C([0, T], C^\infty(\mathbb{R}^n) \cap L^1(\mathbb{R}^n))$;
 - (2) $\psi \in C([0, T], C^\infty(\mathbb{R}^n \setminus \{0\}) \cap L_{loc}^1(\mathbb{R}^n))$.
- (A3) There exists a radial function $\Psi(|\mathbf{k}|) \in L_{loc}^1(\mathbb{R}^n)$, such that $|\psi(\mathbf{k}, t)| \leq \Psi(|\mathbf{k}|)$ in $\mathbb{R}^n \setminus \{0\}$ and $\Psi(|\mathbf{k}|) \leq C_{n,\alpha} |\mathbf{k}|^{-n+\alpha}$ holds for sufficiently large $|\mathbf{k}|$ with given constants $C_{n,\alpha}$ and $\alpha \in (0, n)$.

The prototypes for the second condition in (A2) include several typical nonlocal models, e.g., quantum molecular systems, anomalous diffusions [20, 22], and fractional derivate in financial modeling [30]. Taking the potential $V(\mathbf{x}) = |\mathbf{x} - \mathbf{x}_A|^{-1}$ for $\mathbf{x} \in \mathbb{R}^3$ as an example, we have $\mathbf{z}(\mathbf{x}) = \mathbf{x} - \mathbf{x}_A$ and $\psi(\mathbf{k}) \propto |\mathbf{k}|^{-2}$ with singularities at $\mathbf{k} = 0$ and $\mathbf{k} = \infty$. This motivates us to consider including singular symbols instead of solely treating them in the classical symbol class $C([0, T], S^0(\mathbb{R}^n \times \mathbb{R}^n))$.

In order to distinguish between the weighted-particle (w) and signed-particle (s) models, we replace X_t in (2.4) by X_t^m associated with probability laws Π_Q^m , and we denote by $\Pi_Q^m f(X_t^m)$ the expectation of $f(X_t^m)$ with respect to the probability measure Π_Q^m for $m = w, s$. Theorem 1 estimates the variances of WBRW-HJD.

THEOREM 1 (variances of WBRW-HJD). *Suppose (A1)–(A3) are satisfied, and let $\gamma_1 = 2K_V \gamma_0 + 2\xi^2$. Then the variances of X_t^w and X_t^s satisfy*

$$(2.10) \quad \|\Pi_Q^w(X_t^w - \varphi(t))^2\|_1 \leq \left(1 + \frac{\gamma_1}{\gamma_0}(T-t)\right) e^{2\max(K_V, \frac{\xi^2}{\gamma_0})(T-t)} \|\varphi_T\|_2^2 - \|\varphi(t)\|_2^2,$$

$$(2.11) \quad \|\Pi_Q^s(X_t^s - \varphi(t))^2\|_1 \leq \left(1 + \frac{\gamma_1}{\gamma_0}(T-t)\right) e^{2\xi(T-t)} \|\varphi_T\|_2^2 - \|\varphi(t)\|_2^2.$$

Two key observations are readily made from Theorem 1. One is that the exponential rate for the signed-particle WBRW-HJD is 2ξ , which depends on R and thus

cannot be improved. This poses a huge challenge for high-dimensional problems since ξ usually depends on n exponentially. In contrast, the rate for the weighted-particle WBRW-HJD can be reduced by increasing γ_0 , and the optimal exponential rate is $2K_V$. More precisely, K_V is usually far less than ξ ; this is implied by (2.1) and (2.9). In this sense, the latter outperforms the former. The other observation is that the large exponential rates $2\xi^2/\gamma_0$ and 2ξ , introduced by HJD (1.8), lead to a rapid growth of variance. Such a phenomenon is called the “numerical sign problem” [25], as the HJD of a signed measure totally ignores the near-cancellation of positive and negative weights.

The second contribution of this work is formulating WBRW-SPA in order to diminish the growth of variances. As discussed earlier, our motivation comes from SPA, a useful technique in microlocal analysis [31]. Before proceeding to the variance estimation of WBRW-SPA, we need Theorem 2 to characterize the asymptotic behavior of error terms in SPA.

THEOREM 2 (stationary phase approximation). *Suppose $|\mathbf{z}(\mathbf{x})| \neq 0$ and $\psi \in C([0, T], C_0^\infty(\mathbb{R}^n \setminus \{0\}) \cap L_{loc}^1(\mathbb{R}^n))$. Then for a sufficiently large λ_0 , it holds that*

$$(2.12) \quad \Theta_V[\varphi](\mathbf{x}, \mathbf{k}, t) = \Theta_V^{\lambda_0}[\varphi](\mathbf{x}, \mathbf{k}, t) + \mathcal{O}(\lambda_0^{-n/2}),$$

in the sense that there exists a positive constant C , which depends on ψ and its first derivate but is independent of λ_0 such that

$$(2.13) \quad \|\Theta_V[\varphi](t) - \Theta_V^{\lambda_0}[\varphi](t)\|_2 \leq C\lambda_0^{-n/2}\|\varphi(t)\|_{L_x^2 \times H_k^1}.$$

Here $\|\varphi(t)\|_{L_x^2 \times H_k^1} = \|\varphi(t)\|_2 + \|\nabla_{\mathbf{k}}\varphi(t)\|_2$.

Intuitively speaking, we can use the resulting nonlocal operator $\Theta_V^{\lambda_0}$ to directly formulate WBRW-SPA, instead of using Θ_V as adopted in WBRW-HJD. Specifically, we still use HJD to deal with $\Lambda^{\leq \lambda_0}$ and tackle $\Lambda_+^{> \lambda_0} + \Lambda_-^{> \lambda_0}$ by another two branches of particles, yielding two stochastic processes: the weighted-particle WBRW-SPA and the signed-particle WBRW-SPA. Here we abuse earlier notation X_t^w and X_t^s associated with probability measures Π_Q^w and Π_Q^s , respectively. We further need an enhanced version of (A1), i.e., (A4), plus the extra assumption (A5).

- (A4) $\varphi \in C([0, T], L^2(\mathbb{R}^n) \times H^1(\mathbb{R}^n))$ and is localized in (\mathbf{x}, \mathbf{k}) -space for any $t \in [0, T]$ with the minimal compact support denoted by $\mathcal{X} \times \mathcal{K} \subset \mathbb{R}^n \times \mathbb{R}^n$.
- (A5) For the positive constant ξ in (2.1) there exist positive constants $\lambda_0 > 1$ and $\alpha_* < 1$ such that

$$(2.14) \quad \alpha_* \xi = \max_{0 \leq t \leq T} \max_{\mathbf{x} \in \mathcal{X}} \int_{\mathbb{R}^n} V_W^\pm(\mathbf{x}, \mathbf{k}, t) \mathbb{1}_{\{\mathbf{k} \in \mathbb{R}^n : |2\mathbf{k}| < \lambda_0/|\mathbf{z}(\mathbf{x})|\}}(\mathbf{k}) d\mathbf{k}.$$

Assumption (A5) indicates that the normalizing bound for V_W^\pm can be diminished when \mathbf{k} is restricted in a smaller domain, and this bound holds if $\min_{\mathbf{x} \in \mathcal{X}} |\mathbf{z}(\mathbf{x})|$ is large enough. For instance, it requires the displacement $\min_{\mathbf{x} \in \mathcal{X}} |\mathbf{x} - \mathbf{x}_A|$ to be sufficiently large for $V(\mathbf{x}) = |\mathbf{x} - \mathbf{x}_A|^{-1}$. Accordingly, we are able to show that the first moment of WBRW-SPA turns out to be an asymptotic approximation to the solution of (1.1). We also study how X_t^m deviates from the dual Wigner function φ by estimating the second moment (termed “variance” hereafter) and find that, in contrast to (2.10) and (2.11), the exponential rate in the upper bound is suppressed, so that a moderate growth of variance can be achieved. Namely, the numerical sign problem can be alleviated.

THEOREM 3 (properties of WBRW-SPA). *Suppose (A2)–(A5) are satisfied, and let $\gamma_2 = \alpha_* \check{\xi}^2$. Then for a sufficiently large λ_0 , there exist a weighted-particle WBRW-SPA model X_t^w and a signed-particle counterpart X_t^s , respectively, such that*

$$(2.15) \quad \Pi_Q^w X_t^w = \Pi_Q^s X_t^s = \varphi(\mathbf{x}, \mathbf{k}, t) + \mathcal{O}(\lambda_0^{-n/2}),$$

and their variances satisfy

(2.16)

$$\|\Pi_Q^w(X_t^w - \varphi(t))^2\|_1 \lesssim \left(1 + \frac{4\gamma_2}{\gamma_0}(T-t)\right) e^{2\max(K_V, \frac{\alpha_* \check{\xi}^2}{\gamma_0})(T-t)} \|\varphi_T\|_2^2 - \|\varphi(t)\|_2^2,$$

(2.17)

$$\|\Pi_Q^s(X_t^s - \varphi(t))^2\|_1 \lesssim \left(1 + 2 \left(K_V + \frac{\gamma_2}{\gamma_0}\right)(T-t)\right) e^{2\alpha_* \check{\xi}(T-t)} \|\varphi_T\|_2^2 - \|\varphi(t)\|_2^2.$$

3. Variance estimation of WBRW-HJD. The proof of Theorem 1 under, e.g., the weighted-particle setting, follows by two steps. First, we derive the renewal-type integral equations for the mean-field quantities, including the first and second moments of X_t^w , denoted by $\Phi_w^{(1)}(\mathbf{x}, \mathbf{k}, t) = \Pi_Q^w X_t^w$ and $\Phi_w^{(2)}(\mathbf{x}, \mathbf{k}, t) = \Pi_Q^w(X_t^w)^2$, respectively, as well as the variance $\Delta\Phi_w^{(2)}(\mathbf{x}, \mathbf{k}, t) = \Pi_Q^w(X_t^w - \Phi_w^{(1)}(\mathbf{x}, \mathbf{k}, t))^2$. Second, we analyze the bounds for the renewal-type equations of variances and obtain several basic estimates. The extension to the signed-particle model is straightforward and thus skipped to save space. Prior to the proof, we require the following two lemmas.

LEMMA 4 (backward Grönwall's inequality). *Suppose $\beta > 0$ and that u satisfies the integral inequality*

$$(3.1) \quad u(t) \leq \alpha(t) + \left(1 + \frac{\beta}{\gamma_0}\right) \int_t^T d\mathcal{G}(t' - t) u(t').$$

Then

$$(3.2) \quad u(t) \leq \alpha(t) + (\gamma_0 + \beta) \int_t^T e^{\beta(t' - t)} \alpha(t') dt'.$$

Proof. Let $\tilde{u}(t) = e^{-\gamma_0 t} u(t)$, $\tilde{\alpha}(t) = e^{-\gamma_0 t} \alpha(t)$; then we have

$$\tilde{u}(t) \leq \tilde{\alpha}(t) + (\gamma_0 + \beta) \int_t^T \tilde{u}(t') dt'.$$

By Grönwall's inequality, we have

$$(3.3) \quad \tilde{u}(t) \leq \tilde{\alpha}(t) + (\gamma_0 + \beta) \int_t^T e^{\gamma_0(t' - t) + \beta(t' - t)} \tilde{\alpha}(t') dt'.$$

Substituting $\tilde{u}(t)$ and $\tilde{\alpha}(t)$ into (3.3) yields (3.2). \square

LEMMA 5 (a priori L^2 -boundedness). *Suppose $\varphi_T \in L^2(\mathbb{R}^n \times \mathbb{R}^n)$ and that (2.9) holds. Then for a given $T < \infty$, we have*

$$(3.4) \quad \|\varphi(t)\|_2 \leq e^{K_V(T-t)} \|\varphi_T\|_2, \quad t \in [0, T].$$

Proof. By the triangular inequality and extended Minkowski's inequality, we have

$$\begin{aligned}\|\varphi(t)\|_2 &\leq e^{-\gamma_0(T-t)}\|\varphi_T\|_2 + \left\| \int_t^T d\mathcal{G}(t'-t) \left\{ -\frac{\Theta_V[\varphi](t')}{\gamma_0} + \varphi(t') \right\} \right\|_2 \\ &\leq e^{-\gamma_0(T-t)}\|\varphi_T\|_2 + \left(1 + \frac{K_V}{\gamma_0} \right) \int_t^T d\mathcal{G}(t'-t) \|\varphi(t')\|_2.\end{aligned}$$

Thus, using Lemma 4 we arrive at

$$\frac{\|\varphi(t)\|_2}{\|\varphi_T\|_2} \leq e^{-\gamma_0(T-t)} + (\gamma_0 + K_V) \int_t^T e^{K_V(t'-t)-\gamma_0(T-t')} dt' = e^{K_V(T-t)}. \quad \square$$

Proof of Theorem 1. We only consider the weighted-particle setting. To estimate $\Delta\Phi_w^{(2)}(\mathbf{x}, \mathbf{k}, t)$, we start from the fact that

$$(3.5) \quad \Pi_Q^w(X_t^w)^2 = \Pi_Q^w(\mathbb{1}_{E_t}(X_t^w)^2) + \Pi_Q^w(\mathbb{1}_{E_t^c}(X_t^w)^2),$$

where the events are $E_t = \{\tau_0 : t + \tau_0 \geq T\} \cap \Omega$ and $E_t^c = \{\tau_0 : t + \tau_0 < T\} \cap \Omega$. The second term is expanded as

$$\begin{aligned}\Pi_Q^w(\mathbb{1}_{E_t^c}(X_t^w)^2) &= \sum_{i=1}^3 \int_{E_t^c} \left(w_i^2 \int_{\Omega_i} (X_{t+\tau_0}^w)^2(\omega_i) \Pi_{Q_i}^w(d\omega_i) \right) \Pi_Q^w(d\omega) \\ &+ \sum_{i \neq j} \int_{E_t^c} \left((-1)^{i+j} w_i w_j \int_{\Omega_i} X_{t+\tau_0}^w(\omega_i) \Pi_{Q_i}^w(d\omega_i) \int_{\Omega_j} X_{t+\tau_0}^w(\omega_j) \Pi_{Q_j}^w(d\omega_j) \right) \Pi_Q^w(d\omega).\end{aligned}$$

Thus, the second moment $\Pi_Q^w(X_t^w)^2$ satisfies the following renewal-type equation:

$$(3.6) \quad \begin{aligned}\Pi_Q^w(X_t^w)^2 &= e^{-\gamma_0(T-t)} \varphi_T^2(\mathbf{x}(T-t), \mathbf{k}) + \int_0^{T-t} d\mathcal{G}(\tau_0) B_w[\Phi_w^{(2)}](\mathbf{x}(\tau_0), \mathbf{k}, t + \tau_0) \\ &+ \int_0^{T-t} d\mathcal{G}(\tau_0) C(\mathbf{x}(\tau_0), \mathbf{k}, t + \tau_0),\end{aligned}$$

where the operator B_w (the diagonal component) is given by

$$B_w[\Phi_w^{(2)}](\mathbf{x}, \mathbf{k}, t) = \frac{\xi(\mathbf{x}, t)}{\gamma_0^2} \Theta_V^-[\Phi_w^{(2)}](\mathbf{x}, \mathbf{k}, t) + \frac{\xi(\mathbf{x}, t)}{\gamma_0^2} \Theta_V^+[\Phi_w^{(2)}](\mathbf{x}, \mathbf{k}, t) + \Phi_w^{(2)}(\mathbf{x}, \mathbf{k}, t),$$

and the correlated term $C(\mathbf{x}, \mathbf{k}, t)$ reads as

$$C(\mathbf{x}, \mathbf{k}, t) = -\frac{2}{\gamma_0} \Theta_V[\varphi](\mathbf{x}, \mathbf{k}, t) \cdot \varphi(\mathbf{x}, \mathbf{k}, t) - \frac{2}{\gamma_0^2} \Theta_V^-[\varphi](\mathbf{x}, \mathbf{k}, t) \cdot \Theta_V^+[\varphi](\mathbf{x}, \mathbf{k}, t).$$

By the triangular inequality and Young's inequality, we can readily verify that B_w is a bounded operator from $L^1(\mathbb{R}^n) \times L_0^1(\mathbb{R}^n)$ to itself,

$$(3.7) \quad \begin{aligned}\|B_w[\Phi_w^{(2)}](t)\|_1 &\leq \frac{\check{\xi}}{\gamma_0^2} \|\Theta_V^-[\Phi_w^{(2)}](t)\|_1 + \frac{\check{\xi}}{\gamma_0^2} \|\Theta_V^+[\Phi_w^{(2)}](t)\|_1 + \|\Phi_w^{(2)}(t)\|_1 \\ &\leq \left(1 + \frac{2\check{\xi}^2}{\gamma_0^2} \right) \|\Phi_w^{(2)}(t)\|_1.\end{aligned}$$

Also, by the Cauchy–Schwarz inequality, we have

$$(3.8) \quad \begin{aligned} \|C(t)\|_1 &\leq \frac{2}{\gamma_0} \|\Theta_V[\varphi](t)\|_2 \cdot \|\varphi(t)\|_2 + \frac{2}{\gamma_0^2} \|\Theta_V^-[\varphi](t)\|_2 \cdot \|\Theta_V^+[\varphi](t)\|_2 \\ &\leq \frac{2K_V}{\gamma_0} \|\varphi(t)\|_2^2 + \frac{2\xi^2}{\gamma_0^2} \|\varphi(t)\|_2^2. \end{aligned}$$

Next, we analyze the L^1 -boundedness of $\Delta\Phi_w^{(2)}(\mathbf{x}, \mathbf{k}, t)$, which satisfies the following renewal-type equation according to (3.6):

$$(3.9) \quad \begin{aligned} \Delta\Phi_w^{(2)}(\mathbf{x}, \mathbf{k}, t) &= e^{-\gamma_0(T-t)} \varphi_T^2(\mathbf{x}(T-t), \mathbf{k}) - \varphi^2(\mathbf{x}, \mathbf{k}, t) \\ &\quad + \int_0^{T-t} d\mathcal{G}(\tau) (B_w[\varphi^2](\mathbf{x}(\tau), \mathbf{k}, t+\tau) + C(\mathbf{x}(\tau), \mathbf{k}, t+\tau)) \\ &\quad + \int_0^{T-t} d\mathcal{G}(\tau) B_w[\Delta\Phi_w^{(2)}](\mathbf{x}(\tau), \mathbf{k}, t+\tau). \end{aligned}$$

Now, integrating (3.9) in $\mathbb{R}^n \times \mathbb{R}^n$ and using the triangular inequality, extended Minkowski's inequality, and (3.7), we have

$$(3.10) \quad \begin{aligned} \|\Delta\Phi_w^{(2)}(t)\|_1 &\leq e^{-\gamma_0(T-t)} \|\varphi_T\|_2^2 - \|\varphi(t)\|_2^2 + \int_t^T d\mathcal{G}(t'-t) \|C(t')\|_1 \\ &\quad + \left(1 + \frac{2\xi^2}{\gamma_0^2}\right) \int_t^T d\mathcal{G}(t'-t) (\|\Delta\Phi_w^{(2)}(t')\|_1 + \|\varphi(t')\|_2). \end{aligned}$$

In addition, according to (3.7), (3.8), and Lemma 5, we have

$$(3.11) \quad \begin{aligned} \int_t^T d\mathcal{G}(t'-t) \|C(t')\|_1 &\leq \frac{2K_V\gamma_0 + 2\xi^2}{\gamma_0} \int_t^T e^{2K_V(T-t')} e^{-\gamma_0(t'-t)} dt' \cdot \|\varphi_T\|_2^2 \\ &= \frac{(2K_V\gamma_0 + 2\xi^2)(e^{2K_V(T-t)} - e^{-\gamma_0(T-t)})}{(2K_V + \gamma_0)\gamma_0} \|\varphi_T\|_2^2. \end{aligned}$$

Let

$$(3.12) \quad u(t) = \frac{\|\Delta\Phi_w^{(2)}(t)\|_1 + \|\varphi(t)\|_2^2}{\|\varphi_T\|_2^2}, \quad \alpha_0 = \frac{2K_V\gamma_0 + 2\xi^2}{(2K_V + \gamma_0)\gamma_0}.$$

Then (3.10) is cast as

$$(3.13) \quad u(t) \leq \alpha_0 e^{2K_V(T-t)} + (1 - \alpha_0) e^{-\gamma_0(T-t)} + \left(1 + \frac{2\xi^2}{\gamma_0^2}\right) \int_t^T d\mathcal{G}(t'-t) u(t').$$

Using Lemma 4 yields

$$(3.14) \quad u(t) \leq \frac{K_V\gamma_0 + \xi^2}{K_V\gamma_0 - \xi^2} e^{2K_V(T-t)} - \frac{2\xi^2}{K_V\gamma_0 - \xi^2} e^{\frac{2\xi^2}{\gamma_0}(T-t)},$$

where we use the relations

$$\begin{aligned} \left(\gamma_0 + \frac{2\xi^2}{\gamma_0}\right) \int_t^T e^{2K_V(T-t')} e^{\frac{2\xi^2}{\gamma_0}(t'-t)} dt' &= \frac{\gamma_0^2 + 2\xi^2}{2K_V\gamma_0 - 2\xi^2} (e^{2K_V(T-t)} - e^{\frac{2\xi^2}{\gamma_0}(T-t)}), \\ \left(\gamma_0 + \frac{2\xi^2}{\gamma_0}\right) \int_t^T e^{-\gamma_0(T-t')} e^{\frac{2\xi^2}{\gamma_0}(t'-t)} dt' &= e^{\frac{2\xi^2}{\gamma_0}(T-t)} - e^{-\gamma_0(T-t)}. \end{aligned}$$

Consequently, the following L^1 -boundedness of $\|\Delta\Phi_w^{(2)}(t)\|_1$ for $t \in [0, T]$ is obtained:

$$\|\Delta\Phi_w^{(2)}(t)\|_1 \leq \left(\frac{K_V \gamma_0 + \check{\xi}^2}{K_V \gamma_0 - \check{\xi}^2} e^{2K_V(T-t)} - \frac{2\check{\xi}^2}{K_V \gamma_0 - \check{\xi}^2} e^{\frac{2\check{\xi}^2}{\gamma_0}(T-t)} \right) \|\varphi_T\|_2^2 - \|\varphi(t)\|_2^2.$$

Finally, if $K_V \gamma_0 > \check{\xi}^2$, we have

$$\begin{aligned} \frac{\|\Delta\Phi_w^{(2)}(t)\|_1}{\|\varphi_T\|_2^2} &\leq e^{2K_V(T-t)} - \frac{\|\varphi(t)\|_2^2}{\|\varphi_T\|_2^2} + \frac{2\check{\xi}^2}{K_V \gamma_0 - \check{\xi}^2} e^{2K_V(T-t)} (1 - e^{-2(K_V - \frac{\check{\xi}^2}{\gamma_0})(T-t)}) \\ &\leq e^{2K_V(T-t)} - \frac{\|\varphi(t)\|_2^2}{\|\varphi_T\|_2^2} + \frac{4\check{\xi}^2(T-t)}{\gamma_0} e^{2K_V(T-t)}, \end{aligned}$$

so that the variance is governed by the leading term $e^{2K_V(T-t)}$. Otherwise,

$$\begin{aligned} \frac{\|\Delta\Phi_w^{(2)}(t)\|_1}{\|\varphi_T\|_2^2} &\leq e^{\frac{2\check{\xi}^2}{\gamma_0}(T-t)} - \frac{\|\varphi(t)\|_2^2}{\|\varphi_T\|_2^2} + \frac{\check{\xi}^2 + K_V \gamma_0}{\check{\xi}^2 - K_V \gamma_0} e^{\frac{2\check{\xi}^2}{\gamma_0}(T-t)} (1 - e^{-2(\frac{\check{\xi}^2}{\gamma_0} - K_V)(T-t)}) \\ &\leq e^{\frac{2\check{\xi}^2}{\gamma_0}(T-t)} - \frac{\|\varphi(t)\|_2^2}{\|\varphi_T\|_2^2} + \frac{2(\check{\xi}^2 + K_V \gamma_0)(T-t)}{\gamma_0} e^{\frac{2\check{\xi}^2}{\gamma_0}(T-t)}, \end{aligned}$$

so that the variance is governed by the leading term $e^{\frac{2\check{\xi}^2}{\gamma_0}(T-t)}$ instead. Thus, we have completed the proof. \square

4. Properties of WBRW-SPA. The weakness of HJD lies in ignoring the near-cancellation of the positive and negative parts of Ψ DO in its oscillatory integral representation (1.5), leading to a rapid growth of variance in WBRW-HJD. Fortunately, with the help of SPA, the major contribution of the high-frequency component of Ψ DO can be captured by two leading terms of its asymptotic expansion.

Proof of Theorem 2. We start by splitting the wavevector \mathbf{k} into its modulus and orientation parts $\mathbf{k}' = r\sigma$, with the modulus $r = |\mathbf{k}'| > 0$ and the orientation $\sigma = (\sigma_1, \sigma_2, \dots, \sigma_n) \in \mathbb{S}^{n-1}$, where \mathbb{S}^{n-1} denotes the $(n-1)$ -D spherical surface, and by focusing on the high-frequency component

$$(4.1) \quad \Lambda^{>\lambda_0} = \int_{\frac{\lambda_0}{|\mathbf{z}(\mathbf{x})|}}^{+\infty} r^{n-1} dr \int_{\mathbb{S}^{n-1}} d\sigma e^{ir|\mathbf{z}(\mathbf{x})|\mathbf{z}' \cdot \sigma} \psi(r\sigma, t) \Delta_{r\sigma}[\varphi](\mathbf{x}, \mathbf{k}, t),$$

where $\sigma = (\sigma_1, \dots, \sigma_n)$ represents the orientation of $\mathbf{z}(\mathbf{x})$, $\mathbf{z}' = \mathbf{z}/|\mathbf{z}|$ and $d\sigma$ denotes the induced Lebesgue measure on \mathbb{S}^{n-1} . After choosing the equatorial plane normal to \mathbf{z}' , the unit sphere \mathbb{S}^{n-1} can be decomposed into upper and lower hemispheres \mathbb{S}_+^{n-1} and \mathbb{S}_-^{n-1} , respectively, satisfying $\pm \mathbf{z}' \in \mathbb{S}_\pm^{n-1}$. Accordingly, the inner surface integral of the first kind over \mathbb{S}^{n-1} in (4.1) equals the sum of those over \mathbb{S}_+^{n-1} and \mathbb{S}_-^{n-1} . Without loss of generality, it suffices to assume that $\mathbf{z}' = (0, \dots, 0, 1)$, which can be realized by a rotation otherwise. Let us start from the graph

$$\mathbb{S}_\pm^{n-1} = \{\sigma \in \mathbb{R}^n \mid \sigma_n = \pm \phi(\sigma_1, \dots, \sigma_{n-1}), \sigma_i \in [-1, 1], i = 1, \dots, n-1\},$$

with $\phi(\sigma_1, \dots, \sigma_{n-1}) = \sqrt{1 - \sigma_1^2 - \dots - \sigma_{n-1}^2}$. Now we take the surface integral of the first kind over the upper hemisphere as an example. The phase function of the integrand becomes

$$S(\mathbf{x}, r, \sigma_1, \dots, \sigma_{n-1}) = r|\mathbf{z}(\mathbf{x})|\mathbf{z}' \cdot \sigma = r|\mathbf{z}(\mathbf{x})|\phi(\sigma_1, \dots, \sigma_{n-1}).$$

For such a phase function, it can be easily verified that there is only one critical point $\sigma_+ = (0, \dots, 0, 1)$ satisfying $(\nabla_\sigma S)(\sigma_+) = 0$, and the determinant of its Hessian matrix at σ_+ turns out to be

$$\det(\text{Hess}(S)(\sigma_+)) = \det_{1 \leq j, k \leq n-1} \left(\frac{\partial^2 S}{\partial \sigma_j \partial \sigma_k}(\sigma_+) \right) = (-r|\mathbf{z}(\mathbf{x})|)^{n-1}.$$

Consequently, applying the stationary phase method [17, 31] leads directly to

$$\begin{aligned} & \int_{\mathbb{S}_+^{n-1}} e^{iS(\mathbf{x}, r, \sigma)} \psi(r\sigma, t) \Delta_{r\sigma}[\varphi](\mathbf{x}, \mathbf{k}, t) d\sigma \\ &= e^{ir|\mathbf{z}(\mathbf{x})|} \left(\frac{2\pi}{i r |\mathbf{z}(\mathbf{x})|} \right)^{\frac{n-1}{2}} \psi(r\sigma_+, t) \Delta_{r\sigma_+}[\varphi](\mathbf{x}, \mathbf{k}, t) + R_{\sigma_+}(\mathbf{x}, \mathbf{k}, r, t), \end{aligned}$$

the first term of which exactly recovers the integrand of $\Lambda_+^{>\lambda_0}$ in (2.3). That is, the asymptotic of the oscillatory integral over the upper hemisphere is governed by the contribution from the critical point σ_+ .

It remains to estimate the integral of remainders $\int_{\lambda_0/|\mathbf{z}(\mathbf{x})|}^{+\infty} R_{\sigma_\pm}(\mathbf{x}, \mathbf{k}, r, t) r^{n-1} dr$. Since $\psi(\mathbf{k}, t) \in C([0, T], C_0^\infty(\mathbb{R}^n))$ with its support contained in a compact ball $B(R)$, we can replace ψ by $\psi \cdot \chi_{\varepsilon, R}$, where $\chi_{\varepsilon, R}(r)$ is a smooth truncating function on $[\varepsilon, R]$ and $0 < \varepsilon < \lambda_0/|\mathbf{z}(\mathbf{x})|$, to remove the singularities. Now we rewrite $R_{\sigma_+}(\mathbf{x}, \mathbf{k}, r, t)$ as

$$(4.2) \quad R_{\sigma_\pm}(\mathbf{x}, \mathbf{k}, r, t) = a_\pm(\mathbf{x}, r, t) \chi_{\varepsilon, R}(r) \Delta_{r\sigma_\pm}[\varphi](\mathbf{x}, \mathbf{k}, t) + b_\pm(\mathbf{x}, \mathbf{k}, r, t) \chi_{\varepsilon, R}(r),$$

where

$$\begin{aligned} a_\pm(\mathbf{x}, r, t) &= \int_{\mathbb{S}_\pm^{n-1}} e^{ir|\mathbf{z}(\mathbf{x})| \mathbf{z}' \cdot \sigma} \psi(r\sigma, t) d\sigma - e^{\pm ir|\mathbf{z}(\mathbf{x})|} \left(\frac{2\pi}{\pm i r |\mathbf{z}(\mathbf{x})|} \right)^{\frac{n-1}{2}} \psi(r\sigma_\pm, t), \\ b_\pm(\mathbf{x}, \mathbf{k}, r, t) &= \int_{\mathbb{S}_\pm^{n-1}} e^{ir|\mathbf{z}(\mathbf{x})| \mathbf{z}' \cdot \sigma} \psi(r\sigma, t) (\Delta_{r\sigma}[\varphi] - \Delta_{r\sigma_\pm}[\varphi]) d\sigma. \end{aligned}$$

According to Theorem 7.7.14 in [27], there is an estimate for a_\pm that

$$(4.3) \quad |a_\pm(\mathbf{x}, r, t)| \leq C(r|\mathbf{z}(\mathbf{x})|)^{-\frac{n+1}{2}} \leq C\lambda_0^{-\frac{n+1}{2}}.$$

Thus, for the first term in (4.2), we have

$$\left\| \int_{\lambda_0/|\mathbf{z}(\mathbf{x})|}^{+\infty} r^{n-1} a_\pm(\mathbf{x}, r, t) \chi_{\varepsilon, R}(r) \Delta_{r\sigma_\pm}[\varphi](\mathbf{x}, \mathbf{k}, t) dr \right\|_{L_k^2}^2 \leq \frac{2C^2 R^{2n} \lambda_0^{-(n+1)}}{n^2} \|\varphi(t)\|_{L_k^2}^2.$$

For the second term in (4.2), it suffices to consider a sufficiently smooth φ , so that the localization property of oscillatory integrals allows us to only estimate the integral in the neighborhood U^\pm of the stationary phase points $\sigma_\pm = (0, \dots, 0, \pm 1)$. Due to the Morse lemma, there exists a diffeomorphism from U^+ to a small neighborhood of $\mathbf{y}_+ = (0, \dots, 0)$. Indeed, since $\phi(0, \dots, 0) = 1$ and $\nabla\phi(0, \dots, 0) = 0$, we have that

$$\phi(\sigma_1, \dots, \sigma_{n-1}) - 1 = \int_0^1 (1-t) \frac{d^2\phi}{dt^2}(t\sigma_1, \dots, t\sigma_{n-1}) dt = \sum_{i,j} \sigma_i \sigma_j h_{ij}(\sigma_1, \dots, \sigma_{n-1}),$$

where $h_{ij}(\sigma_1, \dots, \sigma_{n-1}) = \int_0^1 (1-t) \partial_{ij}^2 \phi(t\sigma_1, \dots, t\sigma_{n-1}) dt$.

We note that $H = (h_{ij})$ is a symmetric matrix and nonsingular at $(0, \dots, 0)$, and so is in U^+ by continuity; then there exists a nonsingular $n \times n$ matrix $B(\sigma_1, \dots, \sigma_{n-1}) = (b_{ij}(\sigma_1, \dots, \sigma_{n-1}))$ such that $H = B^\tau B$. Therefore, we can introduce the \mathbf{y} -coordinate

$$\mathbf{y} = (y_1, \dots, y_{n-1})^\tau = B(\sigma_1, \dots, \sigma_{n-1})(\sigma_1, \dots, \sigma_{n-1})^\tau$$

so that the phase function turns out to be a quadratic form,

$$S(\mathbf{x}, r, \sigma) = \tilde{S}(\mathbf{x}, r, \mathbf{y}) = r|\mathbf{z}(\mathbf{x})|(1 - y_1^2 - \dots - y_{n-1}^2).$$

By the implicit function theorem, the inverse conversion $\sigma_i = \kappa_i(y_1, \dots, y_{n-1}) \in C^\infty(\mathbb{R}^{n-1})$ also exists, which satisfies $\kappa_i(0, \dots, 0) = 0$. Therefore, we have that

$$\sigma_i = \kappa_i(y_1, \dots, y_{n-1}) = \int_0^1 \frac{d\kappa_i}{dt}(ty_1, \dots, ty_{n-1}) dt = \sum_{j=1}^{n-1} y_j \kappa_{ij}(y_1, \dots, y_{n-1}),$$

with a suitable C^∞ function κ_{ij} that satisfies $\kappa_{ij}(0, \dots, 0) = \frac{\partial \kappa_i}{\partial y_j}(0, \dots, 0)$.

Now we use Taylor's expansion,

$$\begin{aligned} & \varphi\left(\mathbf{x}, \mathbf{k} \pm \frac{r\sigma}{2}, t\right) - \varphi\left(\mathbf{x}, \mathbf{k} \pm \frac{r\sigma_+}{2}, t\right) \\ &= \pm \frac{1}{2} \sum_{i=1}^{n-1} r\sigma_i \left(\frac{\partial \varphi}{\partial k_i} + \frac{\partial \phi}{\partial \sigma_i} \frac{\partial \varphi}{\partial k_n} \right) \left(\mathbf{x}, \mathbf{k} \pm \frac{r\sigma_+}{2}, t \right) + \mathcal{O}(\sigma^2) \\ &= \pm \frac{1}{2} \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} r y_j \kappa_{ij}(y_1, \dots, y_{n-1}) \left(\frac{\partial \varphi}{\partial k_i} + \tilde{\phi}_i \frac{\partial \varphi}{\partial k_n} \right) \left(\mathbf{x}, \mathbf{k} \pm \frac{r\sigma_+}{2}, t \right) + \mathcal{O}(\mathbf{y}^2), \end{aligned}$$

with $\tilde{\phi}_i(y_1, \dots, y_{n-1}) = \frac{\partial \phi}{\partial \sigma_i}(\sigma_1, \dots, \sigma_{n-1})$. Since the estimate

$$\left| \int_{\mathbb{R}^{n-1}} e^{-i\tilde{S}(\mathbf{x}, r, \mathbf{y})} \mathbf{y}^l \tilde{\psi}(r, \mathbf{y}, t) d\mathbf{y} \right| \leq C(r|\mathbf{z}(\mathbf{x})|)^{-\frac{n-1}{2} - \frac{|l|}{2}}$$

holds for any smooth, nonsingular, compactly \mathbf{y} -supported $\tilde{\psi}(r, \mathbf{y}, t)$ and sufficiently large $r|\mathbf{z}(\mathbf{x})|$ (here we adopt the convention that $\mathbf{y}^l = y_1^{l_1} \dots y_{n-1}^{l_{n-1}}$ for $l_1 + \dots + l_{n-1} = l$) [17], one can conclude that the L^2 norm (in the \mathbf{k} -variable) of $b_+(\mathbf{x}, \mathbf{k}, r, t)$ is majorized by

$$\|b_+(\mathbf{x}, \mathbf{k}, r, t)\|_{L^2_k} \leq C(r|\mathbf{z}(\mathbf{x})|)^{-\frac{n}{2}} \|\nabla_{\mathbf{k}} \varphi(t)\|_{L^2_k} + \mathcal{O}\left((r|\mathbf{z}(\mathbf{x})|)^{-\frac{n+1}{2}}\right).$$

Consequently, we arrive at

$$\left\| \int_{\frac{\lambda_0}{|\mathbf{z}(\mathbf{x})|}}^{+\infty} R_{\sigma_+}(\mathbf{x}, \mathbf{k}, r, t) r^{n-1} dr \right\|_{L^2_k} \leq C \lambda_0^{-\frac{n}{2}} \|\varphi(t)\|_{H^1_k} \int_{\frac{\lambda_0}{|\mathbf{z}(\mathbf{x})|}}^R r^{n-1} dr \lesssim \lambda_0^{-\frac{n}{2}} \|\varphi(t)\|_{H^1_k},$$

which implies (2.13). \square

Remark 2. Here we remark on the order $\mathcal{O}(\lambda_0^{-\frac{n}{2}})$ in Theorem 2. In fact, the stationary phase method cannot be directly applied for a linear phase function in (1.5) due to the degeneracy of its Hessian. That is why we can only obtain an asymptotic reduction in the $(n-1)$ -D spherical coordinate, and the leading terms are $\mathcal{O}(\lambda_0^{-\frac{n-1}{2}})$, instead of $\mathcal{O}(\lambda_0^{-\frac{n}{2}})$ stated by Hörmander's theorem.

Now we prove Theorem 3. Replacing $\Psi\text{DO } \Theta_V$ in (1.1) with its SPA $\Theta_V^{\lambda_0}$ yields the renewal-type integral equation

$$(4.4) \quad \begin{aligned} \tilde{\varphi}(\mathbf{x}, \mathbf{k}, t) = & (1 - \mathcal{G}(T-t))\varphi_T(\mathbf{x}(T-t), \mathbf{k}) \\ & - \int_t^T d\mathcal{G}(t'-t) \left\{ \frac{\Theta_V^{\lambda_0}[\tilde{\varphi}](\mathbf{x}(t'-t), \mathbf{k}', t')}{\gamma_0} - \tilde{\varphi}(\mathbf{x}(t'-t), \mathbf{k}, t') \right\}, \end{aligned}$$

the solution of which turns out to be the first moment of WBRW-SPA. For the bias term $\varphi - \tilde{\varphi}$, an estimate can be readily obtained using Grönwall's inequality.

Proof of Theorem 3. We first need to prove that $\Phi_w^{(1)}(\mathbf{x}, \mathbf{k}, t) = \tilde{\varphi}(\mathbf{x}, \mathbf{k}, t)$, following the same procedure in [10]. Suppose the event E_t^c occurs; then for the family history $\omega = (Q_0; \omega_1, \dots, \omega_5)$, we have that

$$(4.5) \quad X_t^w(\omega) = \sum_{i=1}^4 (-1)^{i+1} \zeta_i \cdot X_t^w(\omega_i) + X_t^w(\omega_5).$$

Owing to the facts that subfamilies ω_i are mutually independent and that the HJD is $\Lambda^{\leq \lambda_0} = \Lambda_+^{\leq \lambda_0} - \Lambda_-^{\leq \lambda_0}$, for two branches with negative weight corresponding to $i_m = 1, 3$ in (2.7) we have that

$$\begin{aligned} \int_{E_t^c} (-1)^{1+1} \zeta_1 \cdot X_t^w(\omega_1) \Pi_Q^w(d\omega) &= \int_0^{T-t} \frac{\Lambda_-^{\leq \lambda_0}[\Phi_w^{(1)}](\mathbf{x}(\tau), \mathbf{k}, t+\tau)}{\gamma_0} d\mathcal{G}(\tau), \\ \int_{E_t^c} (-1)^{1+3} \zeta_3 \cdot X_t^w(\omega_3) \Pi_Q^w(d\omega) &= \int_0^{T-t} \frac{\Lambda_+^{\leq \lambda_0}[\Phi_w^{(1)}](\mathbf{x}(\tau), \mathbf{k}, t+\tau)}{\gamma_0} d\mathcal{G}(\tau). \end{aligned}$$

The remaining three branches can be tackled in a similar manner, and summing those five branches together recovers $-\Theta_V^{\lambda_0}[\varphi] + \gamma_0 \cdot \varphi$.

The next step is to estimate the upper bounds for the variances. When the assumption (A5) holds, $\Lambda_{\pm}^{\leq \lambda_0}$ is bounded from $L^p(\mathbb{R}^n) \times L_0^p(\mathbb{R}^n)$ to itself by Young's inequality,

$$(4.6) \quad \|\Lambda_{\pm}^{\leq \lambda_0}[\varphi](t)\|_p \leq \alpha_* \check{\xi} \|\varphi(t)\|_p, \quad p = 1, 2.$$

According to (2.7) and (4.5), we have that

$$(4.7) \quad \Pi_Q^w(\mathbb{1}_{E_t^c}(X_t^w)^2) = B_w^{\lambda_0}[\Phi_w^{(2)}](\mathbf{x}(\tau_0), \mathbf{k}, t+\tau_0) + \sum_{i \neq j} C_{ij}^{\lambda_0}(\mathbf{x}(\tau_0), \mathbf{k}, t+\tau_0),$$

where the diagonal operator $B_w^{\lambda_0}$ is

$$B_w^{\lambda_0}[\Phi_w^{(2)}](\mathbf{x}(\tau_0), \mathbf{k}, t+\tau_0) = \sum_{i=1}^5 \int_{\Omega_i} w_i^2 \cdot (X_{t+\tau_0}^w)^2(\omega_i) \Pi_{Q_i}^w(d\omega_i),$$

and the correlation term $C_{ij}^{\lambda_0}$ reads as

$$C_{ij}^{\lambda_0}(\mathbf{x}(\tau_0), \mathbf{k}, t+\tau_0) = (-1)^{i+j} \int_{\Omega_i} w_i X_{t+\tau_0}^w(\omega_i) \Pi_{Q_i}^w(d\omega_i) \int_{\Omega_j} w_j X_{t+\tau_0}^w(\omega_j) \Pi_{Q_j}^w(d\omega_j).$$

Since $|\text{Im}[\zeta(r_3, \mathbf{x}(\tau), t + \tau)]|^2 \leq (2\pi/\lambda_0)^{n-1}$, this yields L^1 -boundedness of $B_w^{\lambda_0}$,

(4.8)

$$\begin{aligned} & \left\| \int_{E_t^c} \left(\int_{\Omega_3} w_3^2 \cdot (X_{t+\tau_0}^w(\omega_3))^2 \Pi_{Q_3}^w(d\omega_3) \right) \Pi_Q^w(d\omega) \right\|_{L_k^1} \\ & \leq \frac{4\check{\eta}}{\gamma_0^2} \left(\frac{2\pi}{\lambda_0} \right)^{n-1} \left\| \int_{\lambda_0/|\mathbf{z}_3|}^R r_3^{n-1} \Psi(r_3) \Phi_w^{(2)} \left(\mathbf{x}(\tau), \mathbf{k} - \frac{r_3 \sigma_+(\mathbf{x}(\tau))}{2}, t + \tau \right) dr_3 \right\|_{L_k^1} \\ & \lesssim \frac{4\check{\eta}^2}{\gamma_0^2} \left(\frac{2\pi}{\lambda_0} \right)^{n-1} \|\Phi_w^{(2)}(\mathbf{x}(\tau), \mathbf{k}, t + \tau)\|_{L_k^1}. \end{aligned}$$

Combining (4.6) and (4.8), we obtain that

$$\|B_w^{\lambda_0}[\Phi_w^{(2)}](t)\|_1 \leq \left(1 + \frac{2\alpha_* \check{\xi}^2}{\gamma_0^2} + \frac{8\check{\eta}^2}{\gamma_0^2} \left(\frac{2\pi}{\lambda_0} \right)^{n-1} \right) \|\Phi_w^{(2)}(t)\|_1.$$

Thus, for a sufficiently large λ_0 (such as $\check{\eta}^2 (\frac{2\pi}{\lambda_0})^{n-1} \ll \check{\xi}^2$), we have that

$$(4.9) \quad \|B_w^{\lambda_0}[\Phi_w^{(2)}](t)\|_1 \lesssim \left(1 + \frac{2\alpha_* \check{\xi}^2}{\gamma_0^2} \right) \|\Phi_w^{(2)}(t)\|_1 + \mathcal{O}(\lambda_0^{-(n-1)}).$$

For the correlated terms, by using Young's inequality and the Cauchy-Schwarz inequality, $C^{\lambda_0}(\mathbf{x}, \mathbf{k}, t) = \sum_{i < j} C_{ij}^{\lambda_0}(\mathbf{x}, \mathbf{k}, t)$ can be estimated by

(4.10)

$$\begin{aligned} \|C^{\lambda_0}(t)\|_1 & \leq \left(\frac{\alpha_*^2 \check{\xi}^2}{\gamma_0^2} + \left(\frac{4\check{\eta}^2}{\gamma_0^2} \left(\frac{2\pi}{\lambda_0} \right)^{\frac{n-1}{2}} + \frac{4K_V \check{\eta}}{\gamma_0^2} + \frac{4\check{\eta}}{\gamma_0} \right) \left(\frac{2\pi}{\lambda_0} \right)^{\frac{n-1}{2}} + \frac{K_V}{\gamma_0} \right) \|\tilde{\varphi}(t)\|_2^2 \\ & \lesssim \left(\frac{\alpha_* \check{\xi}^2}{\gamma_0^2} + \frac{K_V}{\gamma_0} \right) \|\tilde{\varphi}(t)\|_2^2 + \mathcal{O}(\lambda_0^{-\frac{n-1}{2}}). \end{aligned}$$

In addition, since

$$\|\Theta_V^{\lambda_0}[\tilde{\varphi}](t)\|_2 \leq K_V \|\tilde{\varphi}(t)\|_2 + C \lambda_0^{-\frac{n-1}{2}} \|\tilde{\varphi}(t)\|_2,$$

according to Lemma 5 this yields that

$$(4.11) \quad \|\tilde{\varphi}(t)\|_2 \lesssim e^{K_V(T-t)} \|\varphi_T\|_2 + \mathcal{O}(\lambda_0^{-\frac{n-1}{2}}).$$

Combining (4.9), (4.10), and (4.11), we have the following result:

$$\begin{aligned} \|\Delta \Phi_w^{(2)}(t)\|_1 & \lesssim e^{-\gamma_0(T-t)} \|\varphi_T\|_2^2 - \|\tilde{\varphi}(t)\|_2^2 + 2 \int_t^T d\mathcal{G}(t' - t) \|C^{\lambda_0}(t')\|_1 \\ & \quad + \left(1 + \frac{2\alpha_* \check{\xi}^2}{\gamma_0^2} \right) \int_t^T d\mathcal{G}(t' - t) \left\{ \|\Delta \Phi_w^{(2)}(t')\|_1 + \|\tilde{\varphi}(t')\|_2 \right\} + \mathcal{O}(\lambda_0^{-\frac{n-1}{2}}). \end{aligned}$$

Note that by replacing $\check{\xi}$ in (3.10) and (3.14) by $\sqrt{\alpha_*} \check{\xi}$, we can further obtain the following estimate for $\|\Delta \Phi_w^{(2)}(t)\|_1$:

$$(4.12) \quad \begin{aligned} \|\Delta \Phi_w^{(2)}(t)\|_1 & \lesssim \left(\frac{K_V \gamma_0 + \alpha_* \check{\xi}^2}{K_V \gamma_0 - \alpha_* \check{\xi}^2} e^{2K_V(T-t)} - \frac{2\alpha_* \check{\xi}^2}{K_V \gamma_0 - \alpha_* \check{\xi}^2} e^{\frac{2\alpha_* \check{\xi}^2}{\gamma_0}(T-t)} \right) \|\varphi_T\|_2^2 \\ & \quad - \|\tilde{\varphi}(t)\|_2^2 + \mathcal{O}(\lambda_0^{-\frac{n-1}{2}}). \end{aligned}$$

Therefore, for the weighted particle model, we have that

$$(4.13) \quad \|\Delta\Phi_w^{(2)}(t)\|_1 \lesssim \left(1 + \frac{4\alpha_*\xi^2}{\gamma_0}(T-t)\right) e^{2\max(K_V, \frac{\alpha_*\xi^2}{\gamma_0})(T-t)} \|\varphi_T\|_2^2 - \|\tilde{\varphi}(t)\|_2^2 + \mathcal{O}(\lambda_0^{-\frac{n-1}{2}}).$$

Finally, let $\varepsilon(\mathbf{x}, \mathbf{k}, t) = \tilde{\varphi}(\mathbf{x}, \mathbf{k}, t) - \varphi(\mathbf{x}, \mathbf{k}, t)$. According to (1.1) and (4.4), it is easy to verify that $\|\varepsilon(t)\|_2 \leq C\lambda_0^{-n/2} \max_{t \in [0, T]} \|\varphi(t)\|_{L_x^2 \times H_k^1}$ since

$$\begin{aligned} \|\varepsilon(t)\|_2 &\leq \int_t^T d\mathcal{G}(t'-t) \|\Theta_V[\varphi](t') - \Theta_V^{\lambda_0}[\varphi](t')\|_2 + \left(1 + \frac{K_V}{\gamma_0}\right) \int_t^T d\mathcal{G}(t'-t) \|\varepsilon(t')\|_2 \\ &\leq \frac{1 - e^{-\gamma_0(T-t)}}{\lambda_0^{n/2}} \max_{t \in [0, T]} \|\varphi(t)\|_{L_x^2 \times H_k^1} + \left(1 + \frac{K_V}{\gamma_0}\right) \int_t^T d\mathcal{G}(t'-t) \|\varepsilon(t')\|_2 \\ &\leq \frac{(\gamma_0 + K_V)e^{K_V(T-t)}}{K_V \lambda_0^{n/2}} \max_{t \in [0, T]} \|\varphi(t)\|_{L_x^2 \times H_k^1}, \end{aligned}$$

where the second inequality uses the remainder estimate (2.13) in Theorem 2 and the third is derived by Lemma 4.

By extended Minkowski's inequality and the Cauchy-Schwarz inequality, we have

$$\|\Pi_Q^w(X_t^w - \varphi(\mathbf{x}, \mathbf{k}, t))^2\|_1 \leq \|\Delta\Phi_w^{(2)}(t)\|_1^2 + 2\|\Phi_w^{(1)}(t) - \tilde{\varphi}(t)\|_2 \cdot \|\varepsilon(t)\|_2 + \|\varepsilon(t)\|_2^2,$$

where the first term is bounded by (4.13), the second vanishes, and the third is $\mathcal{O}(\lambda_0^{-n})$. Thus, this finalizes the proof of (2.16). \square

A direct application of the WBRW algorithms is to evaluate the quantum observables $\langle \hat{A} \rangle(T)$ (i.e., the inner product problem) at instant T using the dual relation between φ and the Wigner function f . Let A_W be the Weyl symbol of quantum operator \hat{A} , and let f_0 be the initial Wigner function. We have that

$$\langle \hat{A} \rangle(T) = \iint_{\mathbb{R}^n \times \mathbb{R}^n} A_W(\mathbf{x}, \mathbf{k}) f(\mathbf{x}, \mathbf{k}, T) d\mathbf{x} d\mathbf{k} = \iint_{\mathbb{R}^n \times \mathbb{R}^n} \varphi(\mathbf{x}, \mathbf{k}, 0) f_0(\mathbf{x}, \mathbf{k}) d\mathbf{x} d\mathbf{k},$$

where $\varphi(\mathbf{x}, \mathbf{k}, 0)$ can be solved by (1.1) with “initial condition” $\varphi_T = A_W$.

The stochastic interpretation of the inner product problem can be established by an extension of the probability space $(\Omega, \mathcal{F}, \Pi_Q^w)$. We introduce a probability measure

$$d\lambda_0 = f_I(\mathbf{x}, \mathbf{k}) d\mathbf{x} d\mathbf{k}, \quad f_I = |f_0| / \|f_0\|_1;$$

the extended probability space is $(\mathbb{R}^{2n} \times \Omega, \mathbb{R}^{2n} \otimes \mathcal{F}, \lambda_0 \otimes \Pi_Q^w)$, where \mathbb{R}^{2n} is the Borel space on \mathbb{R}^{2n} and $\lambda_0 \otimes \Pi_Q^w$ is the product measure. Therefore, we have

$$\langle \hat{A} \rangle(t) = \lambda_0 \otimes \Pi_Q^w(s \cdot X_t^w) = \iint_{\mathbb{R}^n \times \mathbb{R}^n} s(\mathbf{x}, \mathbf{k}) f_I(\mathbf{x}, \mathbf{k}) \left(\int_{\Omega} X_t^w(\omega) \Pi_Q^w(d\omega) \right) d\mathbf{x} d\mathbf{k},$$

where s is short for the particle sign function $s(\mathbf{x}, \mathbf{k}) = f_0(\mathbf{x}, \mathbf{k}) / f_I(\mathbf{x}, \mathbf{k})$.

According to Theorem 3, it is straightforward to obtain the estimate of corresponding variances $\text{Var}(s \cdot X_t^w) = \lambda_0 \otimes \Pi_Q^w(s \cdot X_t^w - \lambda_0 \otimes \Pi_Q^w(s \cdot X_t^w))^2$.

PROPOSITION 6 (variance estimation for the inner product problem). *Suppose $\|f_I\|_{\infty} < \infty$ and that there exists a positive constant $M_s > 0$ such that $s \leq M_s$ holds almost surely in \mathbb{R}^{2n} . Then*

(1) under assumptions (A1)–(A3), for the weighted-particle WBRW-HJD, we have
(4.14)

$$\text{Var}(s \cdot X_t^w) \leq 2M_s^2 \|f_I\|_\infty \left(1 + \left(K_V + \frac{\xi^2}{\gamma_0} \right) (T-t) \right) e^{2 \max(K_V, \frac{\xi^2}{\gamma_0})(T-t)} \|\varphi_T\|_2^2;$$

(2) under assumptions (A2)–(A5), for the weighted-particle WBRW-SPA, we have

$$(4.15) \quad \text{Var}(s \cdot X_t^w) \lesssim 2M_s^2 \|f_I\|_\infty \left(1 + \frac{4\alpha_* \xi^2}{\gamma_0} (T-t) \right) e^{2 \max(K_V, \frac{\alpha_* \xi^2}{\gamma_0})(T-t)} \|\varphi_T\|_2^2.$$

Proposition 6 implies that the variance of the inner product problem can be reduced by chopping the \mathbf{x} -support into several parts and adopting WBRW-SPA for the region in which the two-body distance $|\mathbf{z}(\mathbf{x})|$ is sufficiently large (as stated in assumption (A5)). In other words, WBRW-SPA significantly ameliorates the numerical sign problem in simulating an interacting quantum particle system when α_* is sufficiently small at a cost of some asymptotic biases.

5. Numerical validation. This section is devoted to the numerical validation of our theoretical results with a two-body quantum system under the Morse potential:

$$(5.1) \quad V(\mathbf{x}) = -2e^{-\kappa(|\mathbf{x}-\mathbf{x}_A|-r_0)} + e^{-2\kappa(|\mathbf{x}-\mathbf{x}_A|-r_0)}.$$

Then the displacement is $\mathbf{z}(\mathbf{x}) = (z_1, z_2) = \mathbf{x} - \mathbf{x}_A$, and the amplitude function reads as

$$(5.2) \quad \psi(\mathbf{k}) = \frac{1}{i\hbar} \left[-\frac{2\kappa e^{\kappa r_0} c_2}{(|\mathbf{k}|^2 + \kappa^2)^{3/2}} + \frac{2\kappa e^{2\kappa r_0} c_2}{(|\mathbf{k}|^2 + 4\kappa^2)^{3/2}} \right].$$

Thus Ψ DO becomes

$$(5.3) \quad \Theta_V[\varphi](\mathbf{x}, \mathbf{k}, t) = -\frac{\kappa e^{\kappa r_0} c_2}{\hbar} \int_0^{2\pi} d\vartheta \int_0^{+\infty} dr \frac{r \sin(2\mathbf{z}(\mathbf{x}) \cdot \mathbf{k}')}{\sqrt{r^2 + (\kappa/2)^2}} \frac{\Delta_{r\sigma}[\varphi](\mathbf{x}, \mathbf{k}, t)}{r^2 + (\kappa/2)^2} \\ + \frac{\kappa e^{2\kappa r_0} c_2}{\hbar} \int_0^{2\pi} d\vartheta \int_0^{+\infty} dr \frac{r \sin(2\mathbf{z}(\mathbf{x}) \cdot \mathbf{k}')}{\sqrt{r^2 + \kappa^2}} \frac{\Delta_{r\sigma}[\varphi](\mathbf{x}, \mathbf{k}, t)}{r^2 + \kappa^2},$$

where $\mathbf{k}' = r\sigma = (r \cos \vartheta, r \sin \vartheta)$ and $c_2 = \Gamma(3/2)\pi^{-3/2} \approx 0.1592$. The variances can be monitored within the implementation of WBRW in [24]. The initial condition is chosen to be the Gaussian wavepacket,

$$(5.4) \quad f_0(x_1, x_2, k_1, k_2) = \frac{1}{\pi^2} e^{-0.5(x_1-8)^2 - 0.5(x_2-12)^2 - 2(k_1-0.5)^2 - 2(k_2+0.5)^2}.$$

Other parameters are $\mathbf{x}_A = (10, 10)$, $r_0 = 0.5$, $\kappa = 0.5$, $\hbar = m = 1$, $T = 2$. We measure the variance with the reference solutions produced by the advective-spectral-mixed scheme [32] and display numerical results of such two-body system in 4-D phase space in Figure 1.

Figure 1(a) makes a comparison between the weighted-particle (wp-HJD) and signed-particle (sp-HJD) WBRW-HJDs. The variance of the weighted-particle model can be reduced by choosing a larger γ_0 , while this does not hold for the signed-particle counterpart [10]. Figure 1(b) compares the WBRW-HJD and WBRW-SPA when $\lambda_0 = 8$. It is readily seen that the variances of both the weighted-particle WBRW-SPA (wp-SPA) and the signed-particle counterpart (sp-SPA) are diminished

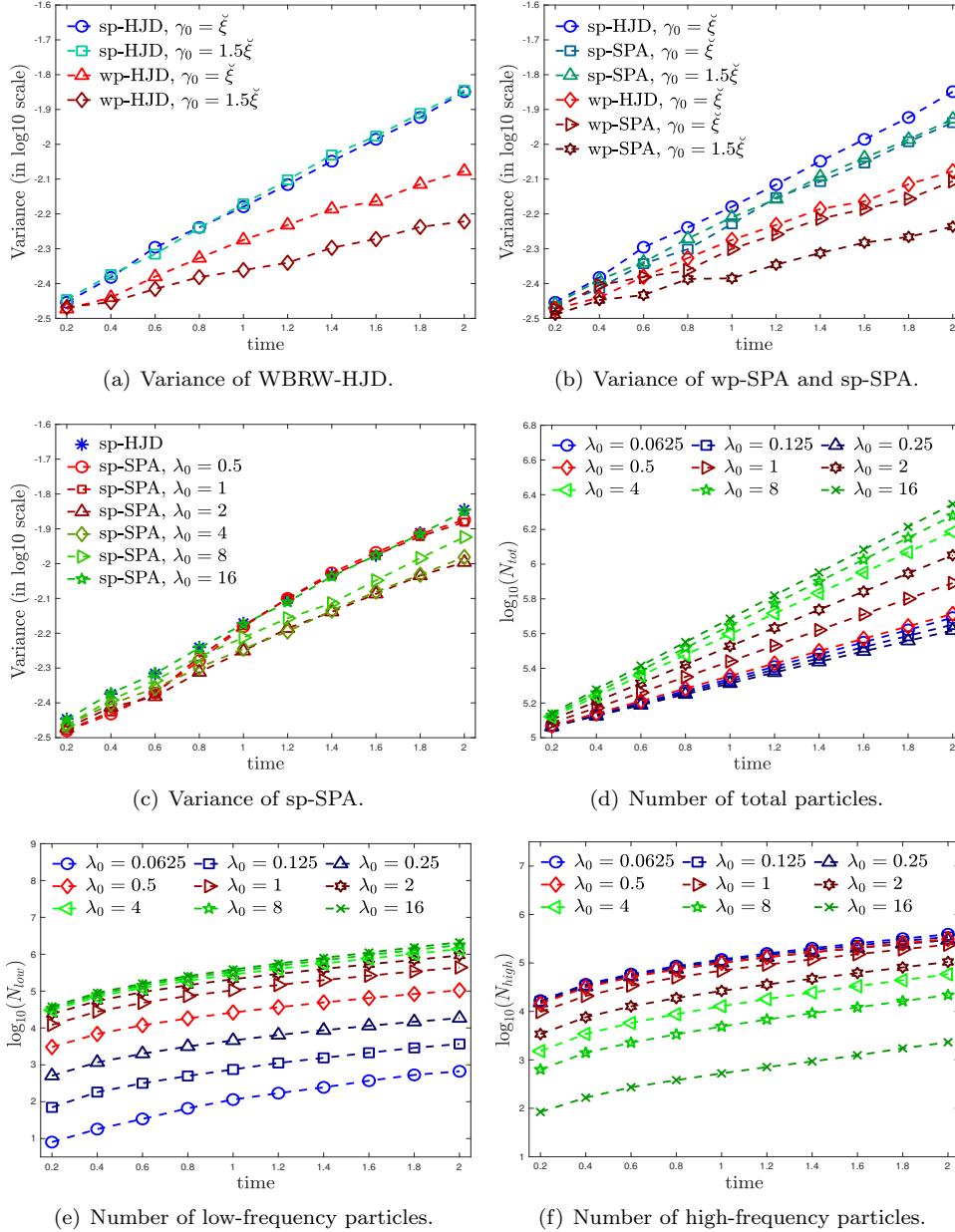


FIG. 1. A two-body Morse system in 4-D phase space: The variance and the number of particles against time, both of which evidently show the exponential growth, are presented. The choice of constant intensity γ_0 has a great influence on the variance of both the weighted-particle WBRW-HJD (wp-HJD) and WBRW-SPA (wp-SPA), while it has little influence on that of the signed-particle counterparts (sp-HJD and sp-SPA). The variances are clearly reduced when SPA is adopted, but the results are not very satisfactory when λ_0 is either too large or too small. This trend coincides with the growth of total particle number N_{tot} , as well as N_{low} and N_{high} corresponding to low-frequency and high-frequency components divided by the filter λ_0 , respectively. Too large λ_0 fails to kill redundant particles effectively, while too small λ_0 leads to an underestimation of N_{low} and a redundancy in N_{high} .

when SPA is adopted, while those of the signed-particle model are still independent of the choice of γ_0 . Figure 1(c) compares sp-SPA under different settings of λ_0 . It is found that the reduction of variance might not be significant for too large λ_0 , as α_* may be very close to 1, and little improvement is also seen for $\lambda_0 \leq 1$ because the asymptotic error dominates for too small λ_0 .

Figures 1(d)–1(f) collect the total particle number N_{tot} , set to be 10^5 initially, and the counts of particles produced from the low-frequency component (N_{low}) and the high-frequency one (N_{high}). The growth of particles coincides with that of variances. Under different choices of λ_0 , N_{tot} always grows exponentially, but the growth rates are distinct. N_{tot} attains its minimum at $\lambda_0 = 0.25$, but further reducing λ_0 leads to a reversal instead. This is because of an overestimation of the asymptotic reduction of the high-frequency component, but, in fact, the asymptotic error $\mathcal{O}(\lambda_0^{-n/2})$ is no longer small. In practice, a guideline for choosing an appropriate λ_0 is to strike a balance between the variance and bias, which may be done by monitoring the growth of N_{low} and N_{high} . One can see that N_{low} must maintain a certain level (see $\lambda_0 \geq 2$) to accurately capture the relevant quantum effects from the low-frequency component, whereas N_{high} cannot be too large; otherwise, it will cause a redundancy in particles (see $\lambda_0 \leq 1$).

6. Conclusion and discussion. In this paper, we have analyzed two classes of branching random walk (BRW) solutions to the Wigner (W) equation, including WBRW-HJD based on the Hahn–Jordan decomposition (HJD), $\Theta_V = \Theta_V^+ - \Theta_V^-$, and WBRW-SPA based on the stationary phase approximation (SPA). The main idea is to split the nonlocal operator with antisymmetric kernels into two parts and explain each of them as the generator of jump process of one branch of weighted particles. We have shown that although the first moment of WBRW-HJD recovers the solution of the Wigner equation, the L^1 -bounds for the variances grow exponentially in time with the rate depending on the norm of Θ_V^\pm , which is inconsistent with the decay rate of the pseudodifferential operator. In contrast, the WBRW-SPA is able to capture the essential contributions from the localized parts, and the variance of the resulting stochastic model can be diminished at the cost of introducing a little bias. These results are of great importance in applications, such as tackling a general form of nonlocal problems. In particular, it ameliorates the numerical sign problem in a high-dimensional situation, which may involve multiple pairs of potentials and high-dimensional oscillatory integrals. Our ongoing work is to apply WBRW-SPA to quantum dynamics under the Coulomb interaction, such as in the hydrogen atom.

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