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A random cloud model for the Wigner equation

Wolfgang Wagner

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Weierstrass Institute
Mohrenstrasse 39
10117 Berlin, Germany
E-Mail: wolfgang.wagner@wias-berlin.de

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Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

A probabilistic model for the Wigner equation is studied. The model is based on a particle system with the time evolution of a piecewise deterministic Markov process. Each particle is characterized by a real-valued weight, a position and a wave-vector. The particle position changes continuously, according to the velocity determined by the wave-vector. New particles are created randomly and added to the system. The main result is that appropriate functionals of the process satisfy a weak form of the Wigner equation.

Contents

1 Introduction

The following facts were established by Eugene Wigner in 1932 [16]. Let ψ be a solution of the Schrödinger equation

$$i\,\hbar\,\frac{\partial}{\partial t}\,\psi(t,x) = -\frac{\hbar^2}{2m}\,\Delta_x\,\psi(t,x) + V(x)\,\psi(t,x)\,, \qquad t \ge 0\,, \quad x \in \mathbb{R}^d\,,$$

where i is the imaginary unit, $\hbar$ is Planck's constant (divided by 2π), m is mass, Δ denotes the Laplace operator, V is potential energy, and $\mathbb{R}^d$ is the d-dimensional Euclidean space. Consider the function

$$f(t,x,k) = \frac{1}{\pi^d}\int_{\mathbb{R}^d} \psi(t,x+y)^*\,\psi(t,x-y)\,\exp(2\,i\,k\cdot y)\,dy\,, \qquad k \in \mathbb{R}^d\,,$$

where the symbols $*$ and $\cdot$ denote the complex conjugate and the scalar product, respectively. Under some restrictions on ψ , the function f has the property

$$\int_{\mathbb{R}^d} f(t,x,k)\,dk = |\psi(t,x)|^2 \qquad \forall\, t \ge 0\,, \quad x \in \mathbb{R}^d\,.$$

Moreover, it satisfies the equation

$$\frac{\partial}{\partial t}\,f(t,x,k) + \frac{\hbar}{m}\,k\cdot\nabla_x\,f(t,x,k) = \int_{\mathbb{R}^d} V_W(x,k-\tilde{k})\,f(t,x,\tilde{k})\,d\tilde{k}\,, \tag{1.1}$$

where

$$V_W(x,k) = \frac{1}{i\,\hbar\,(2\pi)^d}\int_{\mathbb{R}^d} \exp(-i\,k\cdot y)\,\left[V\left(x+\frac{y}{2}\right) - V\left(x-\frac{y}{2}\right)\right]dy \tag{1.2}$$

and ∇ denotes the gradient. The function f is real-valued, but not necessarily non-negative.

Existence and uniqueness issues for the Wigner equation (1.1) were studied, e.g., in [5, 4]. In recent years there has been a growing interest in modelling quantum transport in nanoelectronic devices [9]. In this context, the Wigner equation turned out to be convenient, since it can be coupled easily to the scattering part of the semiconductor Boltzmann equation. A Wigner Monte Carlo method has been developed (see, e.g., [6, 13]), which is based on random systems of positive and negative particles. Several algorithms used in that method are covered by the model introduced in this paper. More specific comments will be given in the concluding section.

This paper is concerned with the construction of a probabilistic model for the Wigner equation (1.1). The model is based on a particle system with the time evolution of a piecewise deterministic Markov process [2]. Each particle is characterized by a real-valued weight, a position $x \in \mathbb{R}^d$ and a wave-vector $k \in \mathbb{R}^d$. The particle position changes continuously, according to the velocity determined by the wave-vector. New particles are created randomly and added to the system. The main result is that appropriate functionals of the process satisfy a weak form of the Wigner equation. Related ideas have been applied previously to the Schrödinger equation in [15].

The paper is organized as follows. The model, the main theorem and the proof are presented in Section 2. Special cases and examples are considered in Section 3. Finally, some comments are given in Section 4.

2 Results

In this section, first the probabilistic model is introduced. It is based on a particle system with a random time evolution depending on several parameters. Then the main theorem is formulated. It establishes an equation satisfied by certain functionals of the stochastic process. This equation is determined by the parameters of the process. It has a more general form compared to the Wigner equation (1.1). This generality indicates the properties of the kernel (1.2), which are essential for the result. Finally, the proof is given. It is based on the theory of piecewise deterministic Markov processes as presented in [2].

2.1 Model

Consider a stochastic process

$$\bar{Z}(t) \quad = \quad \Big(z_j(t) = (u_j(t), x_j(t), k_j(t))\,, \quad j = 1, \ldots, N(t)\Big), \qquad t \geq 0\,, \tag{2.1}$$

with the state space

$$\mathcal{Z} = \cup_{N=1}^{\infty} \mathbb{Z}^N\,.$$

The single particle state space is

$$\mathbb{Z} = \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d\,, \tag{2.2}$$

where the first component represents a weight, the second component is a position vector, and the third component is a wave-vector. Let

$$\bar{z} = (z_1, \ldots, z_N) \in \mathcal{Z}\,, \qquad z = (u, x, k) \in \mathbb{Z}\,. \tag{2.3}$$

The time evolution of the process (2.1) is determined by a flow $\bar{F}$ and a jump kernel Q . Starting at state $\bar{z} \in \mathcal{Z}$, the process performs a deterministic motion according to $\bar{F}$. The random waiting time τ until the next jump satisfies

$$\mathbb{P}(\tau \geq t) = \exp\left(-\int_0^t \lambda(\bar{F}(s, \bar{z}))\, ds\right), \qquad t \geq 0\,,$$

where $\mathbb{P}$ denotes the probability measure and

$$\lambda(\bar{z}) = Q(\bar{z}, \mathcal{Z})\,. \tag{2.4}$$

Then the process jumps into a new state $\bar{\kappa} \in \mathcal{Z}$ distributed according to

$$\frac{1}{\lambda(\bar{F}(\tau, \bar{z}))}\, Q(\bar{F}(\tau, \bar{z}), d\bar{\kappa})\,. \tag{2.5}$$

specification of the flow

We consider the flow

$$\bar{F}(t,\bar{z}) \;=\; \Big(F(t,z_1),\ldots,F(t,z_N)\Big), \qquad t\ge 0\,, \qquad \bar{z}\in\mathcal{Z}\,, \tag{2.6}$$

so that particles move independently of each other. The single particle flow F is

$$F(t,z) \;=\; (u, x+v(k)\,t, k)\,, \qquad t\ge 0\,, \qquad z\in\mathbb{Z}\,, \tag{2.7}$$

where $v(k)$ denotes the velocity corresponding to k . The flow (2.7) satisfies the equation

$$\frac{d}{dt}\,F(t,z) \;=\; (0,v(k),0)\,, \qquad F(0,z)=z\,. \tag{2.8}$$

specification of the jump kernel

We consider jump kernels

$$Q(\bar{z},d\bar{\kappa}) = \sum_{j=1}^{N}\int_{\mathcal{Z}} q(z_j,d\bar{z}')\,\delta_{J(\bar{z};\bar{z}')}(d\bar{\kappa})\,, \qquad \bar{z}\in\mathcal{Z}\,, \tag{2.9}$$

where

$$J(\bar{z};\bar{z}') = (z_1,\ldots,z_N,z_1',\ldots,z_k')\,, \qquad \bar{z}'=(z_1',\ldots,z_k')\in\mathcal{Z}\,, \tag{2.10}$$

and the kernel q will be specified later. The intensity (2.4) takes the form

$$\lambda(\bar{z}) \;=\; \sum_{j=1}^{N} q(z_j,\mathcal{Z})\,. \tag{2.11}$$

A jump according to $Q(\bar{z},d\bar{\kappa})/\lambda(\bar{z})$ is generated as follows. With probabilities

$$\frac{q(z_j,\mathcal{Z})}{\lambda(\bar{z})}\,, \qquad j=1,\ldots,N\,,$$

the j-th particles creates “offspring” $\bar{z}'\in\mathcal{Z}$ distributed according to

$$\frac{1}{q(z_j,\mathcal{Z})}\,q(z_j,d\bar{z}')\,.$$

The new state is

$$\bar{\kappa} = J(\bar{z};\bar{z}')\in\mathcal{Z}\,,$$

where the jump transformation (2.10) adds the offspring to the system.

2.2 Theorem

Let the parameters of the stochastic process (2.1) satisfy the following assumptions.

- The initial state $\bar{Z}(0)$ is such that

$$\mathbb{E}\left(N(0) \max_{j=1,\dots,N(0)} |u_j(0)|\right) \quad < \quad \infty\,, \tag{2.12}$$

  where $\mathbb{E}$ denotes mathematical expectation.

- The velocity field

$$v(k) \quad \text{is locally Lipschitz continuous.} \tag{2.13}$$

- The offspring-creation kernel q has the following properties.
  - The individual offspring-creation rates are bounded, i.e.,

$$q(z, \mathcal{Z}) \quad \le \quad C_q \qquad \forall\, z \in \mathbb{Z}\,, \tag{2.14}$$

    for some constant C_q .
  - The number of offspring (created during a single jump) is bounded, i.e.,

$$q(z, \mathcal{Z}) \quad = \quad q(z, \mathcal{Z}_K) \qquad \forall\, z \in \mathbb{Z}\,, \tag{2.15}$$

    for some $K = 1, 2, \dots$, where

$$\mathcal{Z}_K \quad = \quad \cup_{N=1}^K \mathbb{Z}^N\,.$$

  - The absolute weights of the offspring do not exceed the absolute weight of the parent particle, i.e.,

$$q(z, \mathcal{Z}) \quad = \quad q(z, \mathcal{Z}(z)) \qquad \forall\, z \in \mathbb{Z}\,, \tag{2.16}$$

    where (cf. (2.3))

$$\mathcal{Z}(z) \quad = \quad \left\{\bar{z} \in \mathcal{Z} \;:\; \max_{j=1,\dots,N} |u_j| \le |u|\right\}.$$

Consider some measurable function G on $\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d$ and the class $\mathcal{M}(G)$ of bounded measurable functions φ on $\mathbb{R}^d \times \mathbb{R}^d$ such that

$$\varphi(x, k) \quad \text{is differentiable with respect to} \quad x\,, \tag{2.17}$$

$$\sup_{x,k \in \mathbb{R}^d} |v(k) \cdot (\nabla_x \varphi)(x, k)| \quad < \quad \infty \tag{2.18}$$

and

$$\sup_{x,k \in \mathbb{R}^d} \int_{\mathbb{R}^d} |G(x, k, \tilde{k})\, \varphi(x, \tilde{k})|\, d\tilde{k} \quad < \quad \infty\,. \tag{2.19}$$

Theorem 2.1 *Consider the empirical measures of the process (2.1),*

$$\mu(t,dz) = \sum_{j=1}^{N(t)} \delta_{z_j(t)}(dz)\,, \tag{2.20}$$

and denote

$$\nu(t,dz) = \mathbb{E}\,\mu(t,dz)\,. \tag{2.21}$$

Let the assumptions (2.12)-(2.16) be fulfilled. If q *is such that*

$$\begin{aligned} & u \int_{\mathbb{R}^d} G(x,k,\tilde{k})\,\varphi(x,\tilde{k})\,d\tilde{k} = \\ & \qquad \int_{\mathcal{Z}} \Big[u_1\,\varphi(x_1,k_1) + \ldots + u_N\,\varphi(x_N,k_N)\Big] q(z,dz_1,\ldots,dz_N)\,, \end{aligned} \tag{2.22}$$

for all $z=(u,x,k)\in\mathbb{Z}$ *and* $\varphi\in\mathcal{M}(G)$ *(cf. (2.17)–(2.19)), then the measure-valued functions*

$$f(t,dx,dk) = \int_{\mathbb{R}} u\,\nu(t,du,dx,dk) \tag{2.23}$$

satisfy the equation

$$\begin{aligned} & \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x,k)\,f(t,dx,dk) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x,k)\,f(0,dx,dk) + \\ & \qquad \int_0^t \left(\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \Big[v(k)\cdot(\nabla_x\,\varphi)(x,k)\Big] f(s,dx,dk)\right) ds + \\ & \qquad \int_0^t \left(\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \left[\int_{\mathbb{R}^d} G(x,k,\tilde{k})\,\varphi(x,\tilde{k})\,d\tilde{k}\right] f(s,dx,dk)\right) ds\,, \end{aligned} \tag{2.24}$$

for any $t\geq 0$ *and* $\varphi\in\mathcal{M}(G)$ *.*

According to (2.20), (2.21) and (2.23), one obtains

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x,k)\,f(t,dx,dk) \;=\; \mathbb{E}\left(\sum_{j=1}^{N(t)} u_j(t)\,\varphi(x_j(t),k_j(t))\right). \tag{2.25}$$

Thus, the process (2.1) provides a probabilistic representation for the solution of equation (2.24).

In the following, we provide some straightforward choices for the initial state $\bar{Z}(0)$ and the offspring-creation kernel q , which satisfy the assumptions of Theorem 2.1. The special case of the Wigner equation (1.1), as well as further examples of kernels q , will be discussed in Section 3

initial state

Consider a function $f_0 \in L^1(\mathbb{R}^d \times \mathbb{R}^d)$ and a probability density π on $\mathbb{R}^d \times \mathbb{R}^d$ such that

$$\pi(x,k) > 0 \qquad \forall\, x,k \in \mathbb{R}^d \times \mathbb{R}^d \;:\quad |f_0(x,k)| > 0\,.$$

Let $N(0) = 1$. Generate $x_1(0)$ and $k_1(0)$ according to π . Under the conditions $x_1(0) = x$ and $k_1(0) = k$, define

$$u_1(0) \quad = \quad \frac{f_0(x,k)}{\pi(x,k)}\,.$$

Then assumption (2.12) concerning the initial state is satisfied, since

$$\mathbb{E}\,|u_1(0)| = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} |f_0(x,k)|\, dk\, dx =: \|f_0\|_1 \quad < \quad \infty\,.$$

The simplest choice is $\pi \sim |f_0|$. In this case, one obtains

$$u_1(0) \quad = \quad \|f_0\|_1 \,\mathrm{sign}\, f_0(x,k)\,.$$

offspring-creation kernel

The main assumption (2.22) concerning the offspring-creation kernel q is satisfied for the choice

$$q(z,d\bar z) \quad = \quad \int_{\mathbb{R}^d} d\tilde k\, |G(x,k,\tilde k)|\, \delta_{(u\, sign\, G(x,k,\tilde k),x,\tilde k)}(d\bar z)\,. \tag{2.26}$$

Assumptions (2.15) (with $K = 1$) and (2.16) are also fulfilled. Assumption (2.14) takes the form

$$\sup_{x,k\in\mathbb{R}^d} \int_{\mathbb{R}^d} |G(x,k,\tilde k)|\, d\tilde k \quad < \quad \infty \tag{2.27}$$

and provides a restriction on G . According to the kernel (2.26), a particle $z = (u,x,k)$ creates one offspring

$$\Big(u\,\mathrm{sign}\, G(x,k,\tilde k), x, \tilde k\Big),$$

where $\tilde k$ is distributed according to the density

$$\frac{1}{q(z,\mathcal{Z})}\, |G(x,k,\tilde k)|\,.$$

conservation property

If the function G satisfies (2.27) and

$$\int_{\mathbb{R}^d} G(x,k,\tilde k)\, d\tilde k \quad = \quad 0 \qquad \forall\, x,k \in \mathbb{R}^d\,, \tag{2.28}$$

then the test function $\varphi = 1$ belongs to $\mathcal{M}(G)$ and equation (2.24) implies

$$f(t,\mathbb{R}^d,\mathbb{R}^d) \quad = \quad f(0,\mathbb{R}^d,\mathbb{R}^d) \qquad \forall\, t \ge 0\,. \tag{2.29}$$

2.3 Proof

Step 1: Assumptions **(2.14)** and **(2.15)** imply that, for any $\bar{z} \in \mathcal{Z}$, the "standard" conditions are satisfied:

- the intensity (2.11) is measurable and such that

$$t \to \lambda(\bar{F}(t,\bar{z})) = \sum_{j=1}^{N} q(F(t,z_j),\mathcal{Z}) \quad \text{is integrable on finite intervals;} \tag{2.30}$$

- the process is regular, i.e.,

$$\mathbb{E}_{\bar{z}}\, \#\{l : T_l \leq t\} < \infty \qquad \forall\, t > 0\,, \tag{2.31}$$

  where (T_l) is the sequence of jump times, $\#B$ denotes the number of elements in a set B, and $\mathbb{E}_{\bar{z}}$ is the conditional expectation with respect to the initial state.

Indeed, it follows from (2.14) that

$$\lambda(\bar{z}) \quad \leq \quad C_q\, N \qquad \forall\, \bar{z} \in \mathcal{Z}\,, \tag{2.32}$$

which implies (2.30). According to (2.15), the expected number of jumps of the process (2.1) does not exceed the expected number of jumps of the pure jump process with jumps $N \to N + K$ and intensity $\hat{\lambda}(N) = C_q\, N$. Regularity for the pure jump process follows from the criterion (cf., e.g., [1, p.337])

$$\mathbb{P}_N \left(\sum_{l=0}^{\infty} \frac{1}{\hat{\lambda}(\zeta_l)} = \infty \right) \quad = \quad 1 \qquad \forall\, N = 1,2,\ldots\,,$$

where $\zeta_l = N + l\, K$ is the embedded Markov chain.

It follows from (2.31) and the estimate

$$N(t) \quad \leq \quad N(0) + K\, \#\{l \,:\, T_l \leq t\}$$

that

$$\mathbb{E}_{\bar{z}}\, N(t) \quad < \quad \infty \qquad \forall\, t > 0\,, \quad \bar{z} \in \mathcal{Z}\,. \tag{2.33}$$

Step 2: According to [2, Theorem 26.14], the domain $\mathcal{D}(\mathcal{A})$ of the extended generator of the process (2.1) consists of all measurable functions Ψ such that, for any $\bar{z} \in \mathcal{Z}$,

$$t \to \Psi(\bar{F}(t,\bar{z})) \quad \text{is absolutely continuous} \tag{2.34}$$

and

$$\mathbb{E}_{\bar{z}} \left(\sum_{l:\, T_l \leq \sigma_n} \left| \Psi(\bar{Z}(T_l)) - \Psi(\bar{Z}(T_l-)) \right| \right) < \infty \qquad \forall\, n = 1,2,\ldots\,, \tag{2.35}$$

for some sequence of stopping times $\sigma_n \nearrow \infty$. The extended generator has the form (cf. (2.8))

$$(\mathcal{A}\,\Psi)(\bar{z}) \;=\; \sum_{j=1}^{N} v(k_j)\cdot(\nabla_{x_j}\,\Psi)(\bar{z}) + \int_{\mathcal{Z}} [\Psi(\bar{\kappa}) - \Psi(\bar{z})]\, Q(\bar{z}, d\bar{\kappa})\,. \tag{2.36}$$

For any $\Psi \in \mathcal{D}(\mathcal{A})$, the process

$$M_t(\Psi) = \Psi(\bar{Z}(t)) - \Psi(\bar{z}) - \int_0^t (\mathcal{A}\,\Psi)(\bar{Z}(s))\, ds\,, \qquad t \ge 0\,, \tag{2.37}$$

is a local martingale.

If

$$\mathbb{E}_{\bar{z}} \sup_{s\in[0,t]} |\Psi(\bar{Z}(s))| < \infty \qquad \forall\, t > 0\,, \quad \bar{z} \in \mathcal{Z}\,, \tag{2.38}$$

and

$$\mathbb{E}_{\bar{z}} \sup_{s\in[0,t]} |(\mathcal{A}\,\Psi)(\bar{Z}(s))| < \infty \qquad \forall\, t > 0\,, \quad \bar{z} \in \mathcal{Z}\,, \tag{2.39}$$

then the process (2.37) is a martingale and one obtains the Dynkin formula

$$\mathbb{E}_{\bar{z}}\, \Psi(\bar{Z}(t)) \;=\; \Psi(\bar{z}) + \mathbb{E}_{\bar{z}} \int_0^t (\mathcal{A}\,\Psi)(\bar{Z}(s))\, ds \qquad \forall\, t > 0\,, \quad \bar{z} \in \mathcal{Z}\,. \tag{2.40}$$

If

$$\mathbb{E}\,|\Psi(\bar{Z}(t))| < \infty \qquad \forall\, t \ge 0\,, \tag{2.41}$$

then (2.40) implies

$$\mathbb{E}\,\Psi(\bar{Z}(t)) \;=\; \mathbb{E}\,\Psi(\bar{Z}(0)) + \mathbb{E}\int_0^t (\mathcal{A}\,\Psi)(\bar{Z}(s))\, ds\,. \tag{2.42}$$

Step 3: Consider functions of the form

$$\Psi(\bar{z}) = \psi(z_1) + \ldots + \psi(z_N)\,, \tag{2.43}$$

where ψ is measurable. We check $\Psi \in \mathcal{D}(\mathcal{A})$ provided that

- $\psi(u, x, k)$ is differentiable with respect to x and
- ψ is either bounded or has the form

$$\psi(u, x, k) \;=\; u\,\varphi(x, k)\,, \tag{2.44}$$

  where φ is bounded.

Condition (2.34) is satisfied, according to (2.6) and (2.7)). In order to check condition (2.35), we note that (cf. (2.5), (2.9))

$$\bar{Z}(T_l)) \;=\; J(\bar{Z}(T_l-);\bar{z}'(l)) \qquad \forall\, l=1,2,\ldots\,, \tag{2.45}$$

where $\bar{z}'(l)$ denotes the offspring created at jump time T_l , and (cf. (2.10))

$$\sum_{l:\,T_l\le t}\Big|\Psi(\bar{Z}(T_l))-\Psi(\bar{Z}(T_l-))\Big| \;=\; \sum_{l:\,T_l\le t}\Big|\Psi(\bar{z}'(l))\Big|. \tag{2.46}$$

If ψ is bounded, then condition (2.35) (with $\sigma_n = n$) is a consequence of (2.31), (2.46) and assumption **(2.15)**. If ψ has the form (2.44), then one obtains

$$|\Psi(\bar{z})| \;\le\; U(\bar{z})\,\|\varphi\|_\infty \qquad \forall\,\bar{z}\in\mathcal{Z}\,, \tag{2.47}$$

where $\|.\|_\infty$ denotes the sup-norm and

$$U(\bar{z}) \;=\; \sum_{j=1}^{N}|u_j|\,. \tag{2.48}$$

According to (2.47), one obtains

$$\sum_{l:\,T_l\le t}\Big|\Psi(\bar{z}'(l))\Big| \le \|\varphi\|_\infty \sum_{l:\,T_l\le t} U(\bar{z}'(l)) \le \|\varphi\|_\infty\, U(\bar{Z}(t)) \qquad \forall\, t>0\,. \tag{2.49}$$

Note that each particle created at some jump time $T_l \le t$ belongs to the system (2.1) at time t , and the norm of its weight remains constant. According to (2.7) and assumption **(2.16)**, one obtains

$$\max_{j=1,\ldots,N(t)}|u_j(t)| \;\le\; \max_{j=1,\ldots,N(0)}|u_j(0)| \qquad \forall\, t>0$$

so that

$$U(\bar{Z}(t)) \;\le\; N(t)\max_{j=1,\ldots,N(0)}|u_j(0)| \qquad \forall\, t>0\,. \tag{2.50}$$

Condition (2.35) (with $\sigma_n = n$) is a consequence of (2.33), (2.46), (2.49) and (2.50).

Step 4: We check that (2.40) holds for the function $\Psi(\bar{z}) = N$. This function has the form (2.43) (with $\psi = 1$) and belongs to $\mathcal{D}(\mathcal{A})$. According to (2.32), (2.36) and assumption **(2.15)**, one obtains

$$|(\mathcal{A}\,\Psi)(\bar{z})| \;\le\; K\,C_q\,N\,. \tag{2.51}$$

Since $N(t)$ is increasing, condition (2.38) follows from (2.33), and condition (2.39) is a consequence of (2.33) and (2.51).

Using (2.40) and (2.51), one obtains

$$\mathbb{E}_{\bar{z}}\,N(t) \;\le\; N + K\,C_q\int_0^t \mathbb{E}_{\bar{z}}\,N(s)\,ds$$

and, according to Gronwall's inequality,

$$\mathbb{E}_{\bar{z}}\, N(t) \quad \leq \quad N\, \exp(K\, C_q\, t) \qquad \forall\, t > 0\,, \quad \bar{z} \in \mathcal{Z}\,, \tag{2.52}$$

which generalizes (2.33).

Step 5: We check that (2.42) holds for functions (2.43), (2.44), where $\varphi \in \mathcal{M}(G)$. These functions belong to $\mathcal{D}(\mathcal{A})$. Conditions (2.38), (2.39) and (2.41) will be treated simultaneously.

According to (2.9), (2.10) and assumption **(2.22)**, the extended generator (2.36) takes the form

$$\begin{aligned}(\mathcal{A}\,\Psi)(\bar{z}) \quad &= \quad \sum_{j=1}^{N} v(k_j)\cdot(\nabla_x\,\psi)(z_j) + \sum_{j=1}^{N}\int_{\mathcal{Z}}[\psi(z'_1)+\ldots+\psi(z'_k)]\, q(z_j, d\bar{z}') \qquad (2.53)\\ &= \quad \sum_{j=1}^{N} u_j\, v(k_j)\cdot(\nabla_x\,\varphi)(x_j,k_j) + \sum_{j=1}^{N} u_j\int_{\mathbb{R}^d}\varphi(x_j,k')\, G(x_j,k_j,k')\, dk'\,.\end{aligned}$$

Thus, one obtains (cf. (2.48))

$$|(\mathcal{A}\,\Psi)(\bar{z})| \quad \leq \quad (C_1 + C_2)\, U(\bar{z}) \qquad \forall\, \bar{z} \in \mathcal{Z}\,, \tag{2.54}$$

where C_1 and C_2 are the expressions on the left-hand sides of (2.18) and (2.19), respectively. Conditions (2.38) and (2.39) are consequences of (2.33), (2.47), (2.49), (2.50) and (2.54). Condition (2.41) follows from (2.47), (2.50), (2.52) and assumption **(2.12)**.

According to (2.20), (2.23) and (2.53), one obtains

$$\begin{aligned}\mathbb{E}\,\Psi(\bar{Z}(t)) \quad &= \quad \mathbb{E}\left(\sum_{j=1}^{N(t)}\psi(z_j(t))\right) = \mathbb{E}\left(\int_{\mathbb{Z}}\psi(z)\,\mu(t,dz)\right)\\ &= \quad \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\varphi(x,k)\, f(t,dx,dk) \qquad (2.55)\end{aligned}$$

and

$$\begin{aligned}\mathbb{E}\,(\mathcal{A}\,\Psi)(\bar{Z}(t)) \quad &= \quad \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(t,dx,dk)\Big[v(k)\cdot(\nabla_x\,\varphi)(x,k)\Big] + \\ &\quad\; \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(t,dx,dk)\left[\int_{\mathbb{R}^d}\varphi(x,k')\, G(x,k,k')\, dk'\right], \qquad (2.56)\end{aligned}$$

for any $t \geq 0$. According to (2.55) and (2.56), equation (2.42) takes the form (2.24).

3 Examples

In this section, first the special case of the Wigner equation (1.1) is discussed. Then two classes of offspring-creation kernels are introduced, which satisfy the assumptions of Theorem 2.1. One class is based on the explicit form of the function V_W , while the other class uses the function V directly. Finally, some specific models are considered, where only a single particle with variable weight is involved.

3.1 Wigner equation

For the choices

$$v(k) \;=\; \frac{\hbar}{m}\,k\,, \qquad k \in \mathbb{R}^d\,,$$

and (cf. (1.2))

$$G(x,k,\tilde{k}) \;=\; V_W(x,\tilde{k}-k)\,, \qquad x,k,\tilde{k} \in \mathbb{R}^d\,,$$

equation (2.24) is a measure-valued (and integrated with respect to time) version of the equation

$$\begin{aligned} &\frac{d}{dt}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x,k)\, f(t,x,k)\,dx\,dk = \\ &\quad \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \left[\frac{\hbar}{m}\,k\cdot(\nabla_x\,\varphi)(x,k)\right] f(t,x,k)\,dx\,dk + \\ &\quad \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \left[\int_{\mathbb{R}^d} \varphi(x,\tilde{k})\,V_W(x,\tilde{k}-k)\,d\tilde{k}\right] f(t,x,k)\,dx\,dk\,, \end{aligned} \tag{3.1}$$

which is a weak form of the Wigner equation (1.1). Assumption (2.13) is satisfied. Condition (2.27) takes the form

$$\sup_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} |V_W(x,k)|\,dk \;<\; \infty\,. \tag{3.2}$$

I do not know if there are any non-trivial choices of V, for which condition (3.2) is satisfied. At least, it does not hold in general, as Example 3.1 illustrates.

Example 3.1 *If*

$$V(x) \;=\; a\,1_{[-\varepsilon,\varepsilon]}(x)\,, \qquad x\in\mathbb{R}\,, \qquad \textit{for some} \quad a,\varepsilon>0\,,$$

then

$$V_W(x,k) \;=\; \frac{2\,a}{\hbar\,\pi\,k}\sin(2k\,x)\,\sin(2k\,\varepsilon)\,, \qquad x,k\in\mathbb{R}\,.$$

Therefore, we introduce the functions

$$V_W^{(c)}(x,k) \;=\; \begin{cases} V_W(x,k)\,, & \text{if} \quad \|k\|\le c\,, \\ 0 & , \ \text{otherwise}\,, \end{cases} \tag{3.3}$$

where $c>0$ is a cutoff parameter. It follows from the definition (1.2) that V_W is anti-symmetric with respect to k, i.e.

$$V_W(x,-k) \;=\; -V_W(x,k)\,, \tag{3.4}$$

and such that

$$\sup_{x,k\in\mathbb{R}^d} |V_W(x,k)| \;\le\; \frac{2}{\hbar\,(2\pi)^d}\int_{\mathbb{R}^d} |V(y)|\,dy\,.$$

Thus, the functions (3.3) are anti-symmetric with respect to k and satisfy

$$\sup_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} |V_W^{(c)}(x,k)|\, dk \quad < \quad \infty \tag{3.5}$$

provided that V is integrable.

Since condition (2.27) is fulfilled for the function

$$G(x,k,\tilde{k}) \quad = \quad V_W^{(c)}(x,\tilde{k}-k)\,, \tag{3.6}$$

the kernel (2.26) satisfies the assumptions of Theorem 2.1. Further examples of offspring-creation kernels will be provided in the subsequent sections. The choice (3.6) corresponds to the Wigner equation (3.1) with a cutoff in the function V_W . The conservation property (2.29) is fulfilled, since condition (2.28) is satisfied.

3.2 Offspring-creation according to V_W

Consider

$$G(x,k,\tilde{k}) \quad = \quad g(x,\tilde{k}-k)\,, \qquad x,k,\tilde{k}\in\mathbb{R}^d\,, \tag{3.7}$$

where the function g satisfies

$$g(x,-k) \quad = \quad -g(x,k) \tag{3.8}$$

and

$$\sup_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} |g(x,k)|\, dk \quad < \quad \infty\,. \tag{3.9}$$

This covers the choice (3.6) (cf. (3.4), (3.5)), which corresponds to the Wigner equation. It follows from (3.8) that

$$g^+(x,k) \quad = \quad g^-(x,-k) \tag{3.10}$$

and

$$\int_{\mathbb{R}^d} g^+(x,k)\, dk = \int_{\mathbb{R}^d} g^-(x,k)\, dk = \frac{1}{2}\int_{\mathbb{R}^d} |g(x,k)|\, dk \quad := \quad \gamma(x)\,, \tag{3.11}$$

where g^+ and g^- denote the positive and negative parts of the function g .

creation of one particle

The kernel (2.26) takes the form

$$q_1(z,d\bar{z}) = \int_{\mathbb{R}^d} d\tilde{k}\, |g(x,\tilde{k}-k)|\, \delta_{(u\, sign\, g(x,\tilde{k}-k),x,\tilde{k})}(d\bar{z})\,. \tag{3.12}$$

It satisfies (cf. (3.8), (3.10))

$$
\begin{aligned}
q_1(z,d\bar z) &= \int_{\mathbb{R}^d} d\tilde k\, |g(x,\tilde k)|\, \delta_{(u\, sign\, g(x,\tilde k),x,k+\tilde k)}(d\bar z) \\
&= \int_{\mathbb{R}^d} d\tilde k\, |g(x,\tilde k)|\, \delta_{(-u\, sign\, g(x,\tilde k),x,k-\tilde k)}(d\bar z) \\
&= \int_{\mathbb{R}^d} d\tilde k\, |g(x,\tilde k)| \Big(p\, \delta_{(u\, sign\, g(x,\tilde k),x,k+\tilde k)}(d\bar z) + (1-p)\delta_{(-u\, sign\, g(x,\tilde k),x,k-\tilde k)}(d\bar z)\Big) \\
&= \int_{\mathbb{R}^d} d\tilde k \Big[g^+(x,\tilde k) + g^-(x,\tilde k)\Big] \delta_{(u\, sign\, g(x,\tilde k),x,k+\tilde k)}(d\bar z) \\
&= \int_{\mathbb{R}^d} d\tilde k\, g^+(x,\tilde k) \Big(\delta_{(u,x,k+\tilde k)}(d\bar z) + \delta_{(-u,x,k-\tilde k)}(d\bar z)\Big),
\end{aligned} \tag{3.13}
$$

for any $p \in [0,1]$. Note that (cf. (3.11))

$$q_1(z,\mathcal{Z}) \;=\; 2\,\gamma(x)\,.$$

According to the kernel (3.12), a particle $z=(u,x,k)$ creates one offspring. This offspring can be generated in various equivalent ways (cf. (3.13)).

Example 3.2 *The offspring is*

$$(u\,\mathrm{sign}\, g(x,\tilde k), x, k+\tilde k) \quad \textit{or} \quad (-u\,\mathrm{sign}\, g(x,\tilde k), x, k-\tilde k)\,,$$

with probabilities p *and* $1-p$ *, respectively, where* $\tilde k$ *is distributed according to*

$$\frac{1}{2\,\gamma(x)}\, |g(x,\tilde k)| \tag{3.14}$$

and $p \in [0,1]$ *.*

Example 3.3 *The offspring is*

$$(u,x,k+\tilde k) \quad \textit{or} \quad (-u,x,k-\tilde k)\,,$$

with equal probabilities, where $\tilde k$ *is distributed according to*

$$\frac{1}{\gamma(x)}\, g^+(x,\tilde k)\,. \tag{3.15}$$

creation of two particles

The kernel

$$q_2(z,d\bar z) = \frac{1}{2}\int_{\mathbb{R}^d} d\tilde k\, |g(x,\tilde k)|\, \delta_{((u\, sign\, g(x,\tilde k),x,k+\tilde k),(-u\, sign\, g(x,\tilde k),x,k-\tilde k))}(d\bar z) \tag{3.16}$$

satisfies the main assumption (2.22) of Theorem 2.1 (cf. (3.13) with $p = \frac{1}{2}$). Assumptions (2.15) (with $K = 2$) and (2.16) are also fulfilled. Assumption (2.14) is a consequence of (3.9). Note that (cf. (3.10))

$$\begin{aligned} & q_2(z, d\bar{z}) = \\ & \qquad \frac{1}{2} \int_{\mathbb{R}^d} d\tilde{k} \Big[g^+(x, \tilde{k}) + g^-(x, \tilde{k}) \Big] \delta_{((u\, sign\, g(x,\tilde{k}),x,k+\tilde{k}),(-u\, sign\, g(x,\tilde{k}),x,k-\tilde{k}))}(d\bar{z}) \\ & = \int_{\mathbb{R}^d} d\tilde{k}\, g^+(x, \tilde{k})\, \delta_{((u,x,k+\tilde{k}),(-u,x,k-\tilde{k}))}(d\bar{z}) \end{aligned} \tag{3.17}$$

and (cf. (3.11))

$$q_2(z, \mathcal{Z}) = \gamma(x)\,.$$

According to the kernel (3.16), a particle $z = (u, x, k)$ creates two offspring. These offspring can be generated in various equivalent ways (cf. (3.17)).

Example 3.4 *The two offspring are*

$$(u \operatorname{sign} g(x, \tilde{k}), x, k + \tilde{k}) \quad \textit{and} \quad (-u \operatorname{sign} g(x, \tilde{k}), x, k - \tilde{k})\,,$$

where $\tilde{k}$ is distributed according to (3.14).

Example 3.5 *The two offspring are*

$$(u, x, k + \tilde{k}) \quad \textit{and} \quad (-u, x, k - \tilde{k})\,,$$

where $\tilde{k}$ is distributed according to (3.15).

3.3 Offspring-creation according to V

Since (cf. (1.2))

$$\begin{aligned} V_W(x,k) &= \frac{1}{\hbar\,(2\pi)^d} \int_{\mathbb{R}^d} dy\, \sin(k \cdot y) \left[V\left(x - \frac{y}{2}\right) - V\left(x + \frac{y}{2}\right) \right] \\ &= \frac{2}{\hbar\,(2\pi)^d} \int_{\mathbb{R}^d} dy\, \sin(k \cdot y)\, V\left(x - \frac{y}{2}\right), \end{aligned}$$

the function (3.6) takes the form (cf. (3.3))

$$\begin{aligned} G(x,k,\tilde{k}) &= \chi_{[0,c]}(\|\tilde{k} - k\|)\, V_W(x, \tilde{k} - k) \\ &= c_0\, \chi_{[0,c]}(\|\tilde{k} - k\|) \int_{\mathbb{R}^d} d\tilde{x}\, \sin((\tilde{k} - k) \cdot \tilde{x})\, V\left(x - \frac{\tilde{x}}{2}\right), \end{aligned} \tag{3.18}$$

where χ_B denotes the indicator function of a set B , and

$$c_0 = \frac{2}{\hbar\,(2\pi)^d}\,. \tag{3.19}$$

creation of one particle

The kernel

$$\tilde{q}_1(z,d\bar{z}) = c_0\int_{\mathbb{R}^d} d\tilde{k}\int_{\mathbb{R}^d} d\tilde{x}\,\chi_{[0,c]}(\|\tilde{k}-k\|)\times \left|\sin((\tilde{k}-k)\cdot\tilde{x})\,V\left(x-\frac{\tilde{x}}{2}\right)\right|\delta_{(u'(u,x,\tilde{k}-k,\tilde{x}),x,\tilde{k})}(d\bar{z})\,, \tag{3.20}$$

where

$$u'(u,x,\tilde{k},\tilde{x}) = u\,\mathrm{sign}\left[\sin(\tilde{k}\cdot\tilde{x})\,V\left(x-\frac{\tilde{x}}{2}\right)\right], \tag{3.21}$$

satisfies the main assumption (2.22) of Theorem 2.1. Assumptions (2.15) (with $K=1$) and (2.16) are also fulfilled. Assumption (2.14) takes the form

$$\tilde{q}_1(z,\mathcal{Z}) = c_0\int_{\mathbb{R}^d} d\tilde{k}\int_{\mathbb{R}^d} d\tilde{x}\,\chi_{[0,c]}(\|\tilde{k}\|)\left|\sin(\tilde{k}\cdot\tilde{x})\,V\left(x-\frac{\tilde{x}}{2}\right)\right| \;\le\; C_q \tag{3.22}$$

and is satisfied, if V is integrable. Note that

$$\begin{aligned}\tilde{q}_1(z,d\bar{z}) &= \\ & c_0\int_{\mathbb{R}^d} d\tilde{k}\int_{\mathbb{R}^d} d\tilde{x}\,\chi_{[0,c]}(\|\tilde{k}\|)\left|\sin(\tilde{k}\cdot\tilde{x})\,V\left(x-\frac{\tilde{x}}{2}\right)\right|\delta_{(u'(u,x,\tilde{k},\tilde{x}),x,k+\tilde{k})}(d\bar{z}) \\ =\;& c_0\int_{\mathbb{R}^d} d\tilde{k}\int_{\mathbb{R}^d} d\tilde{x}\,\chi_{[0,c]}(\|\tilde{k}\|)\left|\sin(\tilde{k}\cdot\tilde{x})\,V\left(x-\frac{\tilde{x}}{2}\right)\right|\delta_{(-u'(u,x,\tilde{k},\tilde{x}),x,k-\tilde{k})}(d\bar{z})\,.\end{aligned} \tag{3.23}$$

According to the kernel (3.20), a particle $z=(u,x,k)$ creates one offspring, which can be generated as follows (cf. (3.23)).

Example 3.6 *The offspring is*

$$(u'(u,x,\tilde{k},\tilde{x}),x,k+\tilde{k})\,,$$

where $\tilde{k}$ and $\tilde{x}$ are distributed according to

$$\frac{c_0}{\tilde{q}_1(z,\mathcal{Z})}\,\chi_{[0,c]}(\|\tilde{k}\|)\left|\sin(\tilde{k}\cdot\tilde{x})\,V\left(x-\frac{\tilde{x}}{2}\right)\right|. \tag{3.24}$$

creation of two particles

The kernel

$$\tilde{q}_2(z,d\bar{z}) = \frac{c_0}{2}\int_{\mathbb{R}^d} d\tilde{k}\int_{\mathbb{R}^d} d\tilde{x}\,\chi_{[0,c]}(\|\tilde{k}\|)\times \left|\sin(\tilde{k}\cdot\tilde{x})\,V\left(x-\frac{\tilde{x}}{2}\right)\right|\delta_{((u'(u,x,\tilde{k},\tilde{x}),x,k+\tilde{k})(-u'(u,x,\tilde{k},\tilde{x}),x,k-\tilde{k}))}(d\bar{z})\,, \tag{3.25}$$

where u' is defined in (3.21), satisfies the main assumption (2.22) of Theorem 2.1 (cf. (3.23)). Assumptions (2.15) (with $K = 2$) and (2.16) are also fulfilled. Assumption (2.14) is a consequence of (3.22), since

$$\tilde{q}_2(z, \mathcal{Z}) = \frac{1}{2}\, \tilde{q}_1(z, \mathcal{Z})\,.$$

According to the kernel (3.25), a particle $z = (u, x, k)$ creates two offspring, which can be generated as follows.

Example 3.7 *The two offspring are*

$$(u'(u, x, \tilde{k}, \tilde{x}), x, k + \tilde{k}) \quad \textit{and} \quad (-u'(u, x, \tilde{k}, \tilde{x}), x, k - \tilde{k})\,,$$

where $\tilde{k}$ and $\tilde{x}$ are distributed according to (3.24).

3.4 Single particle models

Consider G of the form (3.7). The kernel

$$\begin{aligned} q_4(z, d\bar{z}) = \frac{1}{6} \int_{\mathbb{R}^d} d\tilde{k}\, |g(x, \tilde{k})| \times & \qquad (3.26) \\ \Big(2\, \delta_{((-u,x,k),(u\, sign\, g(x,\tilde{k}),x,k+\tilde{k}),(u\, sign\, g(x,\tilde{k}),x,k+\tilde{k}),(u\, sign\, g(x,\tilde{k}),x,k+\tilde{k}))}(d\bar{z}) + & \\ \delta_{((-u,x,k),(u,x,k),(u,x,k),(u,x,k))}(d\bar{z})\Big) & \end{aligned}$$

satisfies the main assumption (2.22) of Theorem 2.1. Indeed, one obtains

$$\begin{aligned} \int_{\mathcal{Z}} q_4(z, dz_1, \ldots, dz_N) \Big[u_1\, \varphi(x_1, k_1) + \ldots + u_N\, \varphi(x_N, k_N)\Big] &= \\ \frac{1}{6} \int_{\mathbb{R}^d} d\tilde{k}\, |g(x, \tilde{k})| \Big[-2\, u\, \varphi(x, k) + & \\ 6\, u\, \mathrm{sign}\, g(x, \tilde{k})\, \varphi(x, k + \tilde{k}) - u\, \varphi(x, k) + 3\, u\, \varphi(x, k)\Big] & \\ = \quad u \int_{\mathbb{R}^d} d\tilde{k}\, g(x, \tilde{k})\, \varphi(x, k + \tilde{k})\,. & \end{aligned}$$

Assumptions (2.15) (with $K = 4$) and (2.16) are also fulfilled. Assumption (2.14) is a consequence of (3.9). Thus, this random cloud model with creation of four particles is covered by Theorem 2.1.

However, the special structure of the kernel (3.26) suggests a simple one-particle process. Instead of creating $(-u, x, k)$ and three identical other particles, the parent particle (u, x, k) is replaced by one other particle with triple weight. This one-particle process is different from the random cloud model, but both processes are equivalent in terms of empirical measures.

More generally, we consider a piecewise deterministic Markov process

$$Z(t) = \Big(u(t), x(t), k(t)\Big), \qquad t \ge 0\,, \qquad (3.27)$$

with the state space (2.2), the flow (2.7) and a jump kernel $\tilde{Q}$. The extended generator (2.36) takes the form

$$(\mathcal{A}\,\psi)(z) = v(k)\cdot(\nabla_x\,\psi)(z) + \int_{\mathbb{Z}} [\psi(z') - \psi(z)]\,\tilde{Q}(z,dz')\,.$$

For the process (3.27), representation (2.25) takes the form

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \varphi(x,k)\,f(t,dx,dk) \quad = \quad \mathbb{E}\Big(u(t)\,\varphi(x(t),k(t))\Big).$$

The jump kernel corresponding to the offspring-creation kernel (3.26) is

$$\tilde{Q}_1(z,dz') = \frac{1}{6}\int_{\mathbb{R}^d} d\tilde{k}\,|g(x,\tilde{k})|\Big(2\,\delta_{(3u\,sign\,g(x,\tilde{k}),x,k+\tilde{k})}(dz') + \delta_{(3u,x,k)}(dz')\Big). \tag{3.28}$$

Note that (cf. (3.8), (3.10))

$$\tilde{Q}_1(z,dz') = \frac{1}{3}\int_{\mathbb{R}^d} d\tilde{k}\,g^+(x,\tilde{k})\,\Big(\delta_{(3u,x,k+\tilde{k})}(dz') + \delta_{(-3u,x,k-\tilde{k})}(dz') + \delta_{(3u,x,k)}(dz')\Big) \tag{3.29}$$

and (cf. (3.11))

$$\tilde{Q}_1(z,\mathbb{Z}) = \gamma(x) = q_4(z,\mathcal{Z})\,.$$

The jump can be generated in various equivalent ways.

Example 3.8 *According to (3.28), the particle (u,x,k) jumps into a new state, which is*

$$(3u\,\mathrm{sign}\,g(x,\tilde{k}),x,k+\tilde{k}) \qquad \text{or} \qquad (3u,x,k)\,,$$

with probabilities $\frac{2}{3}$ and $\frac{1}{3}$, respectively, where $\tilde{k}$ is distributed according to (3.14).

Example 3.9 *According to (3.29), the particle (u,x,k) jumps into a new state, which is*

$$(3u,x,k+\tilde{k})\,, \qquad (-3u,x,k-\tilde{k}) \qquad \text{or} \qquad (3u,x,k)\,,$$

with equal probabilities, where $\tilde{k}$ is distributed according to (3.15).

The kernel (3.28) can be generalized. Assume that a jump kernel satisfies

$$\tilde{Q}(z,\{z'\in\mathbb{Z}\,:\,|u'|\le K\,|u|\} \quad = \quad \tilde{Q}(z,\mathbb{Z}) \qquad \forall\,z\in\mathbb{Z}\,,$$

for some $K=1,2,\ldots$. Then the corresponding piecewise deterministic Markov process can be treated via Theorem 2.1. Instead of replacing a particle $z=(u,x,k)$ by a new particle $z'=(u',x',k')$, a set of offspring is added to the system. This set consists of K identical particles $(u'/K,x',k')$ and the "anti-particle" $(-u,x,k)$. However, a direct proof (without making use of Theorem 2.1) would also be rather straightforward. Assumption (2.22) takes the form

$$\int_{\mathbb{Z}} \tilde{Q}(z,dz')\Big[u'\,\varphi(x',k') - u\,\varphi(x,k)\Big] = u\int_{\mathbb{R}^d} G(x,k,\tilde{k})\,\varphi(x,\tilde{k})\,d\tilde{k}\,. \tag{3.30}$$

For the kernel

$$\tilde{Q}_2(z, dz') = c_1 \int_{\mathbb{R}^d} d\tilde{k}\, |g(x,\tilde{k})| \Big(c_2\, \delta_{(\alpha\, u\, sign\, g(x,\tilde{k}), x, k+\tilde{k})}(dz') + c_3\, \delta_{(\beta\, u, x, k)}(dz') \Big), \quad (3.31)$$

where $c_1, c_2, c_3, \alpha, \beta > 0$, the left-hand side of (3.30) is

$$\begin{aligned} & c_1 \int_{\mathbb{R}^d} d\tilde{k}\, |g(x,\tilde{k})| \times \\ & \qquad \Big(c_2 \Big[(\alpha\, u\, \mathrm{sign}\, g(x,\tilde{k})\, \varphi(x, k+\tilde{k}) - u\, \varphi(x,k) \Big] + c_3 \Big[\beta\, u\, \varphi(x,k) - u\, \varphi(x,k) \Big] \Big) \\ & = \quad c_1 \int_{\mathbb{R}^d} d\tilde{k}\, |g(x,\tilde{k})| \times \\ & \qquad \Big(c_2\, \alpha\, u\, \mathrm{sign}\, g(x,\tilde{k})\, \varphi(x, k+\tilde{k}) + [c_3\, (\beta - 1) - c_2]\, u\, \varphi(x,k) \Big). \end{aligned}$$

Thus, condition (3.30) is satisfied if

$$\beta = 1 + \frac{c_2}{c_3} \qquad \text{and} \qquad \alpha = \frac{1}{c_1\, c_2}\,. \quad (3.32)$$

Note that (cf. (3.11))

$$\tilde{Q}_2(z, \mathbb{Z}) = 2\, c_1\, (c_2 + c_3)\, \gamma(x)\,.$$

The jump can be generated as follows.

Example 3.10 *According to (3.31) and (3.32), the particle (u, x, k) jumps into a new state, which is*

$$(\alpha\, u\, \mathrm{sign}\, g(x,\tilde{k}), x, k+\tilde{k}) \qquad \text{or} \qquad (\beta\, u, x, k)\,,$$

with probabilities $\frac{c_2}{c_2+c_3}$ and $\frac{c_3}{c_2+c_3}$, respectively, where $\tilde{k}$ is distributed according to (3.14). Note that Example 3.8 is obtained for the choice $c_1 = \frac{1}{6}$, $c_2 = 2$, $c_3 = 1$.

A similar approach is possible, which uses the function V directly. Consider G of the form (3.18), (3.19). Condition (3.30) is satisfied for the kernel (cf. (3.21))

$$\begin{aligned} \tilde{Q}_3(z, dz') \quad = \quad & c_0\, c_1 \int_{\mathbb{R}^d} d\tilde{k} \int_{\mathbb{R}^d} d\tilde{x}\, \chi_{[0,c]}(\|\tilde{k}\|) \left| \sin(\tilde{k} \cdot \tilde{x})\, V\left(x - \frac{\tilde{x}}{2}\right) \right| \times \\ & \Big(c_2\, \delta_{(\alpha\, u'(u,x,\tilde{k},\tilde{x}), x, k+\tilde{k})}(dz') + c_3\, \delta_{(\beta\, u, x, k)}(dz') \Big), \end{aligned} \quad (3.33)$$

where $c_1, c_2, c_3 > 0$ and α, β are defined in (3.32).

Example 3.11 *According to (3.33), the particle (u, x, k) jumps into a new state, which is*

$$\left(\alpha\, u\, \mathrm{sign} \left[\sin(\tilde{k} \cdot \tilde{x})\, V\left(x - \frac{\tilde{x}}{2}\right) \right], x, k+\tilde{k} \right) \qquad \text{or} \qquad (\beta\, u, x, k)\,,$$

with probabilities $\frac{c_2}{c_2+c_3}$ and $\frac{c_3}{c_2+c_3}$, respectively, where $\tilde{k}, \tilde{x}$ are distributed according to

$$\frac{c_0\, c_1\, (c_2 + c_3)}{\tilde{Q}_3(z, \mathcal{Z})}\, \chi_{[0,c]}(\|\tilde{k}\|) \left| \sin(\tilde{k} \cdot \tilde{x})\, V\left(x - \frac{\tilde{x}}{2}\right) \right|$$

and

$$\tilde{Q}_3(z, \mathcal{Z}) \quad = \quad c_0\, c_1\, (c_2 + c_3) \int_{\mathbb{R}^d} d\tilde{k} \int_{\mathbb{R}^d} d\tilde{x}\, \chi_{[0,c]}(\|\tilde{k}\|) \left| \sin(\tilde{k} \cdot \tilde{x})\, V\left(x - \frac{\tilde{x}}{2}\right) \right|.$$

4 Comments

Theorem 2.1 presents a probabilistic model for the Wigner equation. The approach is based on the general idea of weighted particle systems.

- In classical direct simulation methods, a non-negative function $f(t,z)$, which satisfies a certain equation, is approximated by a particle system
$$z_j(t)\,, \qquad j=1,\ldots,N(t)\,, \quad t\ge 0\,,$$
via
$$\int \varphi(z)\, f(t,z)\, dz \;\sim\; \frac{1}{N}\sum_{j=1}^{N(t)} \varphi(z_j(t))\,, \qquad t\ge 0\,, \tag{4.1}$$
for appropriate test functions φ. The approximation parameter N is related, for example, to the initial number of particles, or to the average number influx per unit time. The variable z represents the state of a single particle. It consists, for example, of position and velocity in the case of the Boltzmann equation, and of position and size in the case of Smoluchowski's coagulation equation.

- If the function f may take negative or even complex values, then a straightforward generalization of (4.1) is
$$\int \varphi(z)\, f(t,z)\, dz \;\sim\; \sum_{j=1}^{N(t)} u_j(t)\, \varphi(z_j(t))\,, \tag{4.2}$$
where the weights u_j are real- or complex-valued and change in time. Various approaches based on approximations of the form (4.2) have been studied in the literature. For example, positive variable weights were used for the Boltzmann equation in [11, 12] and for Smoluchowski's coagulation equation in [8, 7]. Positive and negative weights were used in the deviational particle approach for the Boltzmann equation, e.g., in [3, 14, 10]. Complex-valued weights were used in the random cloud approach for the Schrödinger equation in [15].

Theorem 2.1 provides the basis for an application of the random cloud model in numerics for the Wigner equation. Indeed, if the initial state is chosen as a system of N independent particles with weights normalized by N, then, by the law of large numbers, corresponding functionals of the empirical measures converge (as $N\to\infty$) to the expectation at the right-hand side of the representation (2.25).

- Some special cases covered by the random cloud model appeared in the literature before. In particular, Examples 3.3, 3.5 and 3.9 were derived (in a different way) and used in the context of the so-called Wigner Monte Carlo method (see, e.g., [6, 9, 13]). We did not discuss specific numerical issues such as the cancellation of particle pairs with opposite signs, the introduction of fictitious jumps, or the splitting of transport and jump mechanisms. We only mention that in the models with creation of two particles the conservation property (cf. (2.29)) holds almost surely and not only on average. This makes the corresponding numerical methods much more stable.

- Other particular cases, which seem to be new, may also be of interest in numerical applications. Example 3.4 uses the function $|V_W|$ instead of V_W^+, which might be convenient. It is not clear, how the standard Wigner Monte Carlo method should work, when the function V_W is not explicitly known. Examples 3.6 and 3.7 are based on the function V, which might be useful in this context. The corresponding processes are also interesting from a conceptual point of view, since they show more directly the influence of V on the random behaviour of the particle system.

Theorem 2.1 is formulated for the measure-valued version (2.24) of the Wigner equation. The paper does not address analytical issues such as existence of densities and uniqueness of solutions. These topics are not essential for our main goal – to provide a probabilistic model for the Wigner equation. Another interesting open issue is the study of the limiting behaviour for $c \to \infty$, where c is the cutoff parameter (cf. (3.3)). It is plausible that

$$\lim_{c\to\infty} \int\int \varphi(x,k)\, f^{(c)}(t,dx,dk) \;=\; \int\int \varphi(x,k)\, f(t,dx,dk)\,,$$

where the solutions of the Wigner equation with and without cutoff are denoted by $f^{(c)}$ and f, respectively. However, exchanging the limit $\lim_{c\to\infty}$ and the expectation $\mathbb{E}$ at the right-hand side of (2.25) does not seem to be possible, since the intensity of jumps in the corresponding piecewise-deterministic Markov process would become not only unbounded, but infinite.

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