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A class of probabilistic models for the Schrödinger equation

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Abstract

A class of stochastic particle models for the spatially discretized time-dependent Schrödinger equation is constructed. Each particle is characterized by a complex-valued weight and a position. The particle weights change according to some deterministic rules between the jumps. The jumps are determined by the creation of offspring. The main result is that certain functionals of the particle systems satisfy the Schrödinger equation. The proofs are based on the theory of piecewise deterministic Markov processes.

Contents

1 Introduction

The time-dependent form of the Schrödinger equation for a single electron is

$$i\,\hbar\,\frac{\partial}{\partial t}\,\Phi(t,x) \quad = \quad -\frac{\hbar^2}{2m}\,\Delta_x\Phi(t,x) - q\,V(x)\,\Phi(t,x)\,, \tag{1.1}$$

where Δ denotes the Laplace operator, m is the electron mass, q is the electron charge, V is the electric potential, $\hbar$ is Planck's constant divided by 2π , and i denotes the imaginary unit. Equation (1.1) was established by Erwin Schrödinger in 1926 [14, 15] and is one of the basic equations in quantum mechanics. It describes the time evolution of the so-called wave-function Φ , which represents the quantum state of the electron.

Probabilistic models for deterministic partial differential equations have a long history. Connections between random walks and difference equations were found in [3]. The basic equations for general drift-diffusion processes were established by Kolmogoroff in [10]. A comprehensive account of stochastic models for elliptic and parabolic equations is provided in [12]. Stochastic particle models for the Boltzmann equation were studied in [11] and [9] (see [13, Section 2.3.3] and [16] for more details). The probabilistic approach to quantum mechanics goes back to Feynman ([5], [6]). Developing Feynman's ideas, Kac introduced integration on the space of trajectories of the Wiener process [8] (see [17] for further comments).

This paper is concerned with the construction of a class of probabilistic models for the spatially discretized one-dimensional Schrödinger equation. The models are based on particle systems with the time evolution of a piecewise deterministic Markov process [4]. Each particle is characterized by a complex-valued weight and a position. The particle weights change according to some deterministic rules between the jumps. The jumps are determined by the creation of offspring. The main result is that certain functionals of the processes satisfy the Schrödinger equation. The "random cloud model" introduced in [17] is a special case of the class of models presented here. In this case the particle weights remain constant so that a pure jump process is obtained. A significant improvement of the models with variable weights is that the boundedness assumption on the potential V is avoided.

The paper is organized as follows. The main results are presented in Section 2. Proofs are given in Section 3. Comments are provided in Section 4.

2 Results

We consider the spatially discretized one-dimensional Schrödinger equation

$$\frac{\partial}{\partial t}\,\Phi^{(\varepsilon)}(t,x) \quad = \quad \frac{i\,\hbar}{2m}\,\Delta_x^{(\varepsilon)}\,\Phi^{(\varepsilon)}(t,x) + \frac{i\,q}{\hbar}\,V(x)\,\Phi^{(\varepsilon)}(t,x)\,, \qquad t>0\,, \tag{2.1}$$

with initial condition

$$\Phi^{(\varepsilon)}(0,x) \quad = \quad \Phi_0^{(\varepsilon)}(x)\,, \qquad x\in\mathbb{R}_\varepsilon\,, \tag{2.2}$$

where

$$\mathbb{R}_\varepsilon \quad = \quad \{\varepsilon\,j\,, \quad j=\ldots,-1,0,1,\ldots\}\,, \qquad \varepsilon>0\,. \tag{2.3}$$

The discrete Laplacian

$$\Delta^{(\varepsilon)} f(x) \quad = \quad \frac{f(x+\varepsilon) - 2\,f(x) + f(x-\varepsilon)}{\varepsilon^2} \tag{2.4}$$

is defined for functions f on $\mathbb{R}$. First we construct a probabilistic solution of equation (2.1), that is, a family of complex-valued random variables such that their expectations satisfy the equation. Then the assumption concerning the initial state is discussed. Finally, several modifications of the basic model are introduced.

2.1 Probabilistic representation

We introduce a piecewise-deterministic Markov process (cf. [4]) of the form

$$\Big(w_j(t), x_j(t)\Big), \qquad j = 1, \ldots, N(t)\,, \qquad t \geq 0\,, \tag{2.5}$$

where $w_j(t)$ are complex-valued weights, $x_j(t) \in \mathbb{R}_\varepsilon$ are particle positions, and $N(t)$ is the number of particles in the system at time t . Particles evolve, independently of each other, according to the following rules.

- Starting from a state (w, x) , the particle waits a random time τ , which satisfies

$$\mathbb{P}(\tau \geq s) \quad = \quad \exp\left(-\frac{\hbar}{m\,\varepsilon^2}\,s\right), \qquad s \geq 0\,. \tag{2.6}$$

- While waiting, the particle position remains the same, but the particle weight changes to the value

$$\tilde{w} \quad = \quad w\,\exp\left(i\left[\frac{q}{\hbar}\,V(x) - \frac{\hbar}{m\,\varepsilon^2}\right]\tau\right). \tag{2.7}$$

- After time τ , the particle creates an offspring of the form

$$\begin{cases} (i\,\tilde{w}, x-\varepsilon)\,, & \text{with probability } \frac{1}{2}\,, \\ (i\,\tilde{w}, x+\varepsilon)\,, & \text{with probability } \frac{1}{2}\,, \end{cases} \tag{2.8}$$

  which is added to the system.

The following theorem provides a probabilistic solution of the Schrödinger equation (2.1).

Theorem 2.1 *Consider the particle system (2.5) and the index sets*

$$\mathbb{N}(t,x) \quad = \quad \Big\{j = 1, \ldots, N(t)\;:\; x_j(t) = x\Big\}\,, \qquad t \geq 0\,, \quad x \in \mathbb{R}_\varepsilon\,. \tag{2.9}$$

Assume that the initial state satisfies

$$\mathbb{E}\left(N(0)\max_{j=1,\ldots,N(0)} |w_j(0)|\right) \quad < \quad \infty\,, \tag{2.10}$$

where $|\zeta| = \sqrt{\zeta_1^2 + \zeta_2^2}$ *denotes the norm of a complex number* $\zeta = \zeta_1 + i\,\zeta_2$ *. Then the function*

$$\Phi^{(\varepsilon)}(t,x) \;=\; \mathbb{E}\left(\sum_{j\in\mathbb{N}(t,x)} w_j(t)\right), \qquad t>0\,, \qquad x\in\mathbb{R}_\varepsilon\,, \tag{2.11}$$

satisfies equation (2.1), with initial condition (2.2) and

$$\Phi_0^{(\varepsilon)}(x) \;=\; \mathbb{E}\left(\sum_{j\in\mathbb{N}(0,x)} w_j(0)\right) \qquad x\in\mathbb{R}_\varepsilon\,. \tag{2.12}$$

2.2 Initial state

Assumption (2.10) implies that the function (2.12) satisfies

$$\|\Phi_0^{(\varepsilon)}\| := \sum_{x\in\mathbb{R}_\varepsilon} |\Phi_0^{(\varepsilon)}(x)| \;<\; \infty\,. \tag{2.13}$$

This follows from the estimate

$$\begin{aligned}
\sum_{x\in\mathbb{R}_\varepsilon} |\Phi_0^{(\varepsilon)}(x)| \;&=\; \sum_{x\in\mathbb{R}_\varepsilon}\left|\mathbb{E}\left(\sum_{j=1}^{N(0)} 1_x(x_j(0))\,w_j(0)\right)\right| \\
&\le\; \sum_{x\in\mathbb{R}_\varepsilon}\mathbb{E}\left(\sum_{j=1}^{N(0)} 1_x(x_j(0)) \max_{k=1,\dots,N(0)}|w_k(0)|\right) \\
&=\; \mathbb{E}\left(\sum_{j=1}^{N(0)} \max_{k=1,\dots,N(0)}|w_k(0)|\right) = \mathbb{E}\left(N(0)\max_{k=1,\dots,N(0)}|w_k(0)|\right),
\end{aligned}$$

where 1_x denotes the indicator function of the set consisting of x .

On the other hand, if some function $\Phi_0^{(\varepsilon)}$ satisfies (2.13), then the initial state

$$\Big(w_j(0), x_j(0)\Big), \qquad j=1,\dots,N(0)\,, \tag{2.14}$$

can be chosen in such a way that conditions (2.10) and (2.12) hold.

- The simplest choice is $N(0)=1$, where $x_1(0)$ is generated according to any distribution π such that

$$\pi(x)>0 \qquad \forall\, x\in\mathbb{R}_\varepsilon\;:\quad |\Phi_0^{(\varepsilon)}(x)|>0 \tag{2.15}$$

and, under the condition $x_1(0)=x$,

$$w_1(0) \;=\; \frac{\Phi_0^{(\varepsilon)}(x)}{\pi(x)}\,. \tag{2.16}$$

Indeed, (2.10) follows from

$$\mathbb{E}\,|w_1(0)| = \sum_{x\in\mathbb{R}_\varepsilon} \mathbb{E}(|w_1(0)|\,|\,x_1(0)=x)\,\mathbb{P}(x_1(0)=x) = \sum_{x\in\mathbb{R}_\varepsilon} |\Phi_0^{(\varepsilon)}(x)|\,, \tag{2.17}$$

while (2.12) is a consequence of

$$\mathbb{E}\Big(w_1(0)\,1_x(x_1(0))\Big) = \mathbb{E}(w_1(0)\,|\,x_1(0)=x)\,\mathbb{P}(x_1(0)=x) = \Phi_0^{(\varepsilon)}(x)\,. \tag{2.18}$$

A particular distribution satisfying (2.15) is

$$\pi(x) \quad = \quad \frac{|\Phi_0^{(\varepsilon)}(x)|}{\|\Phi_0^{(\varepsilon)}\|}\,, \qquad x\in\mathbb{R}_\varepsilon\,,$$

In this case, (2.16) takes the form

$$w_1(0) \quad = \quad \|\Phi_0^{(\varepsilon)}\|\,\frac{\Phi_0^{(\varepsilon)}(x)}{|\Phi_0^{(\varepsilon)}(x)|}\,.$$

- A slightly more general choice uses independent particles (2.14). Consider $N(0)=n$, for some $n=1,2,\ldots$. Let $x_j(0)$ be distributed according to some π satisfying (2.15) and, under the condition $x_j(0)=x$,

$$w_j(0) \quad = \quad \frac{\Phi_0^{(\varepsilon)}(x)}{n\,\pi(x)}\,.$$

In this case, (2.10) follows from

$$\mathbb{E}\left(\max_{j=1,\ldots,n}|w_j(0)|\right) \le \mathbb{E}\left(\sum_{j=1}^{n}|w_j(0)|\right) = n\,\mathbb{E}\,|w_1(0)|$$

and (2.17), while (2.12) is a consequence of

$$\mathbb{E}\left(\sum_{j=1}^{n}1_x(x_j(0))\,w_j(0)\right) = n\,\mathbb{E}\Big(1_x(x_1(0))\,w_1(0)\Big)$$

and (2.16), (2.18).

- Consider $N(0)=2\,n+2$, for some $n=1,2,\ldots$. Let $x_j(0)$, $j=1,\ldots,2\,n+1$, be the elements of the set $\mathbb{R}_\varepsilon\cap[-\varepsilon\,n,\varepsilon\,n]$ and

$$w_j(0) \quad = \quad \Phi_0^{(\varepsilon)}(x_j(0))\,.$$

Define $(w_{2n+2}(0),x_{2n+2}(0))$ as in the first example, with $\Phi_0^{(\varepsilon)}$ replaced by the restriction of $\Phi_0^{(\varepsilon)}$ to the set $\mathbb{R}_\varepsilon\setminus[-\varepsilon\,n,\varepsilon\,n]$. Particles with zero weights are redundant and can be skipped. Conditions (2.10) and (2.12) are fulfilled. Thus, if the function $\Phi_0^{(\varepsilon)}$ has compact support, then a deterministic choice of the initial state (2.14) is possible.

2.3 Modifications

We introduce several other models of the form (2.5), for which Theorem 2.1 holds. First the offspring creation events (2.8) are modified. Then the weight change formula (2.7) is generalized. Denote (cf. (2.6), (2.7))

$$c_1(\varepsilon) = \frac{\hbar}{2\,m\,\varepsilon^2}\,, \qquad c_2(x) = \frac{q}{\hbar}\,V(x)\,. \tag{2.19}$$

model with particle cancellation

All particles at the same location are combined by summing up their weights. Otherwise, the evolution (2.6)-(2.8) is applied.

double-offspring model

Particles evolve, independently of each other, according to the following rules.

- Starting from a state (w, x) , the particle waits a random time τ , which is exponentially distributed with parameter

$$\lambda = c_1(\varepsilon)\,. \tag{2.20}$$

- While waiting, the particle position remains the same, but the particle weight changes to the value

$$\tilde{w} = w\,\exp\Big(i\Big[c_2(x) - 2\,c_1(\varepsilon)\Big]\tau\Big). \tag{2.21}$$

- After time τ , the particle creates the pair of offspring

$$(i\,\tilde{w}, x-\varepsilon)\,,\ (i\,\tilde{w}, x+\varepsilon)\,, \tag{2.22}$$

  which is added to the system.

This evolution can be combined with particle cancellation.

multi-offspring model

Many combinations of offspring are possible. We provide only one extremal example, where particles evolve dependent on each other. Namely, the waiting time parameter for the system is (2.20). The weights change according to (2.21). At jump time, pairs of offspring (2.22) are created for all particles simultaneously.

This evolution can be combined with particle cancellation.

single-offspring models with parameter dependent weight change

The time evolution depends on parameters $\alpha, \beta \in [0,1]$ that determine the level of weight change between the jumps. Particles evolve, independently of each other, according to the following rules.

- Starting from a state (w,x), the particle waits a random time τ, which is exponentially distributed with parameter
$$\lambda \;=\; 2\,(2-\alpha)\,c_1(\varepsilon) + (1-\beta)\,|c_2(x)|\,. \tag{2.23}$$
- While waiting, the particle position remains the same, but the particle weight changes to the value
$$\tilde{w} \;=\; w\,\exp\Big(i\,\Big[\beta\,c_2(x) - 2\,\alpha\,c_1(\varepsilon)\Big]\,\tau\Big). \tag{2.24}$$
- After time τ, the particle creates an offspring of the form
$$\begin{cases} (i\,\tilde{w}, x-\varepsilon)\,, & \text{with probability } \frac{c_1(\varepsilon)}{\lambda}\,,\\ (i\,\tilde{w}, x+\varepsilon)\,, & \text{with probability } \frac{c_1(\varepsilon)}{\lambda}\,,\\ (-i\,\tilde{w}, x)\,, & \text{with probability } \frac{2\,(1-\alpha)\,c_1(\varepsilon)}{\lambda}\,,\\ (i\,\tilde{w}\,\mathrm{sign}\,V(x), x)\,, & \text{with probability } \frac{(1-\beta)\,|c_2(x)|}{\lambda}\,, \end{cases} \tag{2.25}$$
which is added to the system.

Theorem 2.1 holds under the additional assumption
$$(1-\beta)\,|V(x)| \;\le\; V_{\max} \qquad \forall\, x\in\mathbb{R}_\varepsilon\,, \qquad \text{for some} \quad V_{\max} > 0\,. \tag{2.26}$$

In the special case $\alpha = \beta = 1$, the waiting time parameter (2.23) corresponds to (2.6), the weight transformation (2.24) corresponds to (2.7) and the offspring creation procedure (2.25) corresponds to (2.8). In this case, the generation of offspring at the same position is completely included into the variable weight. This corresponds to a minimal number of jumps (creation events) and maximal weight change.

In the special case $\alpha = \beta = 0$, there is no weight change so that the process is a pure jump process with constant weights. This corresponds a maximal number of creation events. If the weights are restricted to the values $1, -1,\ i$ and $-i$, then the model reduces to the original "random cloud model" introduced in [17].

3 Proofs

The proof of Theorem 2.1 and its modifications is based on the theory of piecewise deterministic Markov processes as presented in [4]. First some results from the abstract theory are recalled. Then these results are applied to a particle system under general, but rather implicit, assumptions on the model parameters. Finally the assumptions are checked for various specifications of the parameters.

3.1 General theory

Consider a particle system

$$\bar{Z}(t) \quad = \quad \Big(z_j(t)\,, \quad j = 1, \ldots, N(t)\Big), \qquad t \geq 0\,, \tag{3.1}$$

with the state space

$$\mathcal{Z} \quad = \quad \cup_{N=1}^{\infty} \mathbb{Z}^N\,, \tag{3.2}$$

where $\mathbb{Z} = \mathbb{R}^d$ is the state space of a single particle. Considering a state space with no boundary simplifies the theory of piecewise deterministic Markov processes considerably.

The time evolution of the system is determined by a flow $\bar{F}$ and a jump kernel $\bar{Q}$. Starting at state $\bar{z} \in \mathcal{Z}$, the system (3.1) performs a deterministic motion according to $\bar{F}$. The random waiting time τ until the next jump satisfies

$$\mathbb{P}(\tau \geq t) = \exp\left(-\int_0^t \bar{\lambda}(\bar{F}(s,\bar{z}))\,ds\right), \qquad t \geq 0\,, \tag{3.3}$$

where

$$\bar{\lambda}(\bar{z}) \quad = \quad \bar{Q}(\bar{z}, \mathcal{Z})\,. \tag{3.4}$$

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

$$\frac{1}{\bar{\lambda}(\bar{F}(\tau,\bar{z}))}\,\bar{Q}(\bar{F}(\tau,\bar{z}), d\bar{\kappa})\,. \tag{3.5}$$

The flow

$$\bar{F}: \; [0,\infty) \times \mathcal{Z} \to \mathcal{Z}$$

is supposed to satisfy

$$\bar{F}(t, \mathbb{Z}^N) \subset \mathbb{Z}^N \qquad \forall\, t \geq 0\,, \quad N = 1, 2, \ldots\,.$$

It is defined as the unique solution of the equation

$$\frac{d}{dt}\,\bar{F}(t,\bar{z}) \quad = \quad \bar{g}(\bar{F}(t,\bar{z}))\,, \qquad t > 0\,, \tag{3.6}$$

with initial condition

$$\bar{F}(0,\bar{z}) = \bar{z}\,, \qquad \bar{z} \in \mathcal{Z}\,,$$

where $\bar{g}$ is a sufficiently smooth mapping.

Assume that, for any $\bar{z} \in \mathcal{Z}$, the "standard" conditions are satisfied:

- the intensity (3.4) is measurable and such that

$$t \to \bar{\lambda}(\bar{F}(t,\bar{z})) \quad \text{is integrable on finite intervals;} \tag{3.7}$$

- the jump kernel is measurable and such that

$$\bar{Q}(\bar{z}, \{\bar{z}\}) = 0\,; \tag{3.8}$$

- the process is regular, i.e.,

$$\mathbb{E}_{\bar{z}}\, \#\{k : T_k \le t\} < \infty \qquad \forall\, t > 0\,, \tag{3.9}$$

  where (T_k) 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.

Then, according to [4, Theorem 26.14], the domain $\mathcal{D}(A)$ of the extended generator of the process consists of all measurable functions Ψ such that, for any $\bar{z} \in \mathcal{Z}$,

$$t \to \Psi(\bar{F}(t, \bar{z})) \quad \text{is absolutely continuous} \tag{3.10}$$

and

$$\mathbb{E}_{\bar{z}} \left(\sum_{k:\, T_k \le \sigma_l} \left| \Psi(\bar{Z}(T_k)) - \Psi(\bar{Z}(T_k-)) \right| \right) < \infty \qquad \forall\, l = 1, 2, \ldots\,, \tag{3.11}$$

for some sequence of stopping times $\sigma_l \nearrow \infty$ (e.g., $\sigma_l = T_l$ or $\sigma_l = l$). The extended generator has the form

$$(A\,\Psi)(\bar{z}) \;=\; (\bar{D}\,\Psi)(\bar{z}) + \int_{\mathcal{Z}} [\Psi(\bar{\kappa}) - \Psi(\bar{z})]\, \bar{Q}(\bar{z}, d\bar{\kappa})\,, \tag{3.12}$$

where (cf. (3.6))

$$(\bar{D}\,\Psi)(\bar{z}) \;=\; \sum_{j=1}^{N} \sum_{k=1}^{d} \bar{g}_{j,k}(\bar{z})\, \frac{\partial}{\partial z_{j,k}}\, \Psi(\bar{z}) \tag{3.13}$$

and

$$\bar{z} = (z_1, \ldots, z_N) \in \mathcal{Z}\,, \qquad z_j = (z_{j,1}, \ldots, z_{j,d}) \in \mathbb{Z}\,, \quad j = 1, \ldots, N\,.$$

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

$$M_t(\Psi) = \Psi(\bar{Z}_t) - \Psi(\bar{z}) - \int_0^t (A\,\Psi)(\bar{Z}_s)\, ds\,, \qquad t \ge 0\,, \tag{3.14}$$

is a local martingale.

If

$$\mathbb{E}_{\bar{z}} \sup_{s\in[0,t]} |\Psi(\bar{Z}(s))| < \infty \qquad \forall\, t > 0\,, \quad \bar{z} \in \mathcal{Z}\,, \tag{3.15}$$

and

$$\mathbb{E}_{\bar{z}} \sup_{s\in[0,t]} |(A\,\Psi)(\bar{Z}(s))| < \infty \qquad \forall\, t > 0\,, \quad \bar{z} \in \mathcal{Z}\,, \tag{3.16}$$

then the process (3.14) is a martingale and one obtains the Dynkin formula

$$\mathbb{E}_{\bar{z}}\,\Psi(\bar{Z}(t)) \quad = \quad \Psi(\bar{z}) + \mathbb{E}_{\bar{z}} \int_0^t (A\,\Psi)(\bar{Z}(s))\,ds\,. \tag{3.17}$$

If

$$\mathbb{E}\,|\Psi(\bar{Z}(t))| < \infty \qquad \forall\, t \geq 0\,, \tag{3.18}$$

then (3.17) implies

$$\mathbb{E}\,\Psi(\bar{Z}(t)) \quad = \quad \mathbb{E}\,\Psi(\bar{Z}(0)) + \mathbb{E} \int_0^t (A\,\Psi)(\bar{Z}(s))\,ds\,. \tag{3.19}$$

3.2 Application

Consider a particle system of the form (3.1),

$$\bar{Z}(t) \quad = \quad \Big(z_j(t) = (w_{1,j}(t), w_{2,j}(t), x_j(t))\,, \quad j = 1, \ldots, N(t)\Big), \qquad t \geq 0\,, \tag{3.20}$$

with the state space (3.2). The single particle state space is

$$\mathbb{Z} = \mathbb{R}^2 \times \mathbb{X}\,, \tag{3.21}$$

where the first two components represent scalar weights and $\mathbb{X} = \mathbb{R}$ is the position space. We introduce the corresponding empirical measures

$$\mu(t, dz) = \sum_{j=1}^{N(t)} \delta_{z_j(t)}(dz) = \sum_{j=1}^{N(t)} \delta_{w_{1,j}(t)}(dw_1)\,\delta_{w_{2,j}(t)}(dw_2)\,\delta_{x_j(t)}(dx) \tag{3.22}$$

and define

$$f_1(t, dx) = \int_{\mathbb{R}} w_1\,\nu(t, dw_1, \mathbb{R}, dx)\,, \qquad f_2(t, dx) = \int_{\mathbb{R}} w_2\,\nu(t, \mathbb{R}, dw_2, dx)\,, \tag{3.23}$$

where

$$\nu(t, dz) \quad = \quad \mathbb{E}\,\mu(t, dz)\,, \qquad t \geq 0\,, \qquad z = (w_1, w_2, x) \in \mathbb{Z}\,. \tag{3.24}$$

First we derive an equation satisfied by the functions (3.23).

Lemma 3.1 *Let φ_1, φ_2 denote arbitrary functions on $\mathbb{X}$, which are measurable, bounded and have bounded support. Assume that*

(i) $\bar{Z}(0)$, $\bar{F}$ *and* $\bar{Q}$ *are such that conditions (3.7)-(3.11), (3.15), (3.16) and (3.18) are satisfied for all functions of the form*

$$\Psi(\bar{z}) = \psi(z_1) + \ldots + \psi(z_N)\,, \tag{3.25}$$

where

$$\psi(z) \quad = \quad w_1\,\varphi_1(x) + w_2\,\varphi_2(x)\,, \qquad z = (w_1, w_2, x) \in \mathbb{Z}\,; \tag{3.26}$$

(ii) $\bar{F}$ *and* $\bar{Q}$ *are such that the extended generator (3.12) satisfies (cf. (2.19))*

$$(A\,\Psi)(\bar{z}) = \sum_{j=1}^{N} \Big[c_2(x_j)\,\psi(-w_{2,j}, w_{1,j}, x_j) + \tag{3.27}$$
$$c_1(\varepsilon)\Big(\psi(-w_{2,j}, w_{1,j}, x_j - \varepsilon) + \psi(-w_{2,j}, w_{1,j}, x_j + \varepsilon) + 2\,\psi(w_{2,j}, -w_{1,j}, x_j)\Big)\Big],$$

for any

$$\bar{z} \;=\; \Big(z_j = (w_{1,j}, w_{2,j}, x_j)\,, \quad j = 1, \ldots, N\Big) \in \mathcal{Z} \tag{3.28}$$

and Ψ *of the form (3.25), (3.26).*

Then the measure-valued functions (3.23) satisfy the equation

$$\sum_{y=1}^{2} \int_{\mathbb{X}} \varphi_y(x)\, f_y(t, dx) = \sum_{y=1}^{2} \int_{\mathbb{X}} \varphi_y(x)\, f_y(0, dx) - \int_0^t ds \sum_{y=1}^{2} \int_{\mathbb{X}} \tilde{\varphi}_y(x)\, f_y(s, dx)\,, \tag{3.29}$$

where

$$\tilde{\varphi}_y(x) = \tilde{s}(y)\Big[c_2(x)\,\varphi_{\tilde{y}(y)}(x) + c_1(\varepsilon)\Big(\varphi_{\tilde{y}(y)}(x-\varepsilon) + \varphi_{\tilde{y}(y)}(x+\varepsilon) - 2\,\varphi_{\tilde{y}(y)}(x)\Big)\Big] \tag{3.30}$$

and

$$\tilde{s}(y) \;=\; \begin{cases} -1\,, & \text{if} \quad y = 1\,, \\ 1\,, & \text{if} \quad y = 2\,, \end{cases} \qquad\qquad \tilde{y}(y) \;=\; \begin{cases} 2\,, & \text{if} \quad y = 1\,, \\ 1\,, & \text{if} \quad y = 2\,. \end{cases} \tag{3.31}$$

Proof. It follows from (3.22), (3.25) and (3.26) that

$$\Psi(\bar{Z}(t)) = \int_Z \psi(z)\,\mu(t, dz) = \sum_{j=1}^{N(t)} \Big[w_{1,j}(t)\,\varphi_1(x_j(t)) + w_{2,j}(t)\,\varphi_2(x_j(t))\Big] \tag{3.32}$$

and (cf. (3.23), (3.24))

$$\mathbb{E}\,\Psi(\bar{Z}(t)) = \int_Z \psi(z)\,\nu(t, dz) = \int_{\mathbb{X}} \varphi_1(x)\, f_1(t, dx) + \int_{\mathbb{X}} \varphi_2(x)\, f_2(t, dx)\,. \tag{3.33}$$

According to assumption (*ii*), one obtains

$$(A\,\Psi)(\bar{Z}(t)) = \int_Z \mu(t, dz)\Big[c_2(x)\,\psi(-w_2, w_1, x) +$$
$$c_1(\varepsilon)\Big(\psi(-w_2, w_1, x - \varepsilon) + \psi(-w_2, w_1, x + \varepsilon) + 2\,\psi(w_2, -w_1, x)\Big)\Big]$$

and

$$\mathbb{E}\,(A\,\Psi)(\bar{Z}(t)) = \int_Z \nu(t, dz)\Big[c_2(x)\Big(-w_2\,\varphi_1(x) + w_1\,\varphi_2(x)\Big) +$$

$$
\begin{aligned}
& c_1(\varepsilon)\Big(- w_2\, \varphi_1(x-\varepsilon) + w_1\, \varphi_2(x-\varepsilon) - w_2\, \varphi_1(x+\varepsilon) + w_1\, \varphi_2(x+\varepsilon) + \\
& 2\, w_2\, \varphi_1(x) - 2\, w_1\, \varphi_2(x)\Big)\Big] \\
= \; & \int_{\mathbb{X}} f_2(t,dx)\Big[- c_2(x)\, \varphi_1(x) - c_1(\varepsilon)\Big(\varphi_1(x-\varepsilon) + \varphi_1(x+\varepsilon) - 2\, \varphi_1(x)\Big)\Big] + \\
& \int_{\mathbb{X}} f_1(t,dx)\Big[c_2(x)\, \varphi_2(x) + c_1(\varepsilon)\Big(\varphi_2(x-\varepsilon) + \varphi_2(x+\varepsilon) - 2\, \varphi_2(x)\Big)\Big] \\
= \; & -\sum_{y=1}^{2} \int_{\mathbb{X}} f_y(t,dx)\, \tilde{s}(y)\Big[c_2(x)\, \varphi_{\tilde{y}(y)}(x) + \qquad (3.34) \\
& c_1(\varepsilon)\Big(\varphi_{\tilde{y}(y)}(x-\varepsilon) + \varphi_{\tilde{y}(y)}(x+\varepsilon) - 2\, \varphi_{\tilde{y}(y)}(x)\Big)\Big].
\end{aligned}
$$

According to assumption (*i*), equation (3.19) holds so that (3.29) is a consequence of (3.33) and (3.34). ■

Next we establish equation (2.1).

Corollary 3.2 *Consider the particle system (3.20) and denote*

$$
w_j(t) = w_{1,j}(t) + i\, w_{2,j}(t)\,, \qquad j = 1, \ldots, N(t)\,, \qquad t \geq 0\,. \tag{3.35}
$$

Let the assumptions (i) and (ii) of Lemma 3.1 be fulfilled. Furthermore, assume that

(iii) $\bar{Z}(0)$, $\bar{F}$ *and* $\bar{Q}$ *are such that the particle positions are concentrated on* $\mathbb{R}_\varepsilon$ *(cf. (2.3)).*

Then the corresponding function (2.11) satisfies equation (2.1).

Proof. According to assumption (*iii*), the measures (3.23) are concentrated on $\mathbb{R}_\varepsilon$. The corresponding densities are denoted by the same symbols f_1, f_2 . As a consequence of Lemma 3.1 and equation (3.29), the function

$$
\sum_{y=1}^{2} \sum_{x \in \mathbb{R}_\varepsilon} \varphi_y(x)\, f_y(t,x)\,, \qquad t \geq 0\,, \tag{3.36}
$$

is continuous, for any functions φ_1, φ_2 with bounded support. Since the functions $\tilde{\varphi}_1, \tilde{\varphi}_2$ (cf. (3.30)) have bounded support, it follows from (3.29) that the function (3.36) is differentiable and satisfies the equation

$$
\frac{d}{dt} \sum_{y=1}^{2} \sum_{x \in \mathbb{R}_\varepsilon} \varphi_y(x)\, f_y(t,x) = -\sum_{y=1}^{2} \sum_{x \in \mathbb{R}_\varepsilon} \tilde{\varphi}_y(x)\, f_y(t,x)\,.
$$

Thus, using the property (cf. (3.31))

$$
\tilde{y}(\tilde{y}(y)) = y\,, \qquad \tilde{s}(\tilde{y}(y)) = -\tilde{s}(y)\,, \qquad y = 1, 2\,,
$$

one obtains

$$\frac{d}{dt}\sum_{y=1}^{2}\sum_{x\in\mathbb{R}_\varepsilon}\varphi_y(x)\,f_y(t,x) = \tag{3.37}$$
$$-\sum_{y=1}^{2}\sum_{x\in\mathbb{R}_\varepsilon}\tilde{\varphi}_y(x)\,f_y(t,x) = -\sum_{y=1}^{2}\sum_{x\in\mathbb{R}_\varepsilon}\tilde{\varphi}_{\tilde{y}(y)}(x)\,f_{\tilde{y}(y)}(t,x)$$
$$= \sum_{y=1}^{2}\sum_{x\in\mathbb{R}_\varepsilon}\tilde{s}(y)\Big[c_2(x)\,\varphi_y(x)+c_1(\varepsilon)\Big(\varphi_y(x-\varepsilon)+\varphi_y(x+\varepsilon)-2\,\varphi_y(x)\Big)\Big]f_{\tilde{y}(y)}(t,x)\,.$$

By choosing appropriate test functions, it follows from (3.37) that

$$\frac{\partial}{\partial t}\,f_y(t,x) =$$
$$\tilde{s}(y)\Big\{c_1(\varepsilon)\Big[f_{\tilde{y}(y)}(t,x+\varepsilon)-2\,f_{\tilde{y}(y)}(t,x)+f_{\tilde{y}(y)}(t,x-\varepsilon)\Big]+c_2(x)\,f_{\tilde{y}(y)}(t,x)\Big\}\,,$$

which implies

$$\frac{\partial}{\partial t}\,f_1(t,x) = -c_1(\varepsilon)\Big[f_2(t,x+\varepsilon)-2\,f_2(t,x)+f_2(t,x-\varepsilon)\Big]-c_2(x)\,f_2(t,x) \tag{3.38}$$

and

$$\frac{\partial}{\partial t}\,f_2(t,x) = c_1(\varepsilon)\Big[f_1(t,x+\varepsilon)-2\,f_1(t,x)+f_1(t,x-\varepsilon)\Big]+c_2(x)\,f_1(t,x)\,. \tag{3.39}$$

Since, according to (3.32) and (3.33),

$$\mathbb{E}\,\Psi(\bar{Z}(t)) = \mathbb{E}\sum_{j=1}^{N(t)}\Big[w_{1,j}(t)\,\varphi_1(x_j(t))+w_{2,j}(t)\,\varphi_2(x_j(t))\Big] = \sum_{y=1}^{2}\sum_{x\in\mathbb{R}_\varepsilon}\varphi_y(x)\,f_y(t,x)\,,$$

one obtains (cf. (2.9))

$$f_y(t,x) = \mathbb{E}\sum_{j=1}^{N(t)}w_{y,j}(t)\,\delta_x(x_j(t)) = \mathbb{E}\sum_{j\in\mathbb{N}(t,x)}w_{y,j}(t)\,,\qquad y=1,2\,. \tag{3.40}$$

With the notations (3.35), it follows from (3.38)–(3.40) that the corresponding function (2.11) satisfies

$$\frac{\partial}{\partial t}\,\Phi^{(\varepsilon)}(t,x) = i\,c_1(\varepsilon)\Big[\Phi^{(\varepsilon)}(t,x+\varepsilon)-2\,\Phi^{(\varepsilon)}(t,x)+\Phi^{(\varepsilon)}(t,x-\varepsilon)\Big]+i\,c_2(x)\,\Phi^{(\varepsilon)}(t,x)\,,$$

which is (2.1) (cf. (2.4), (2.19)). ■

3.3 Specifications

According to Corollary 3.2, it remains to provide sufficient conditions for assumptions (i)–(iii) in terms of the initial state $\bar{Z}(0)$, the flow $\bar{F}$ and the jump kernel $\bar{Q}$. Note that

- assumption (i) combines the technical conditions (3.7)-(3.9) (related to the existence of the process), (3.10), (3.11) (related to the domain of the extended generator) and (3.15), (3.16), (3.18) (related to the validity of the Dynkin formula);
- assumption (ii) assures the desired form of the equation;
- assumption (iii) restricts the position space to the spatial grid.

specification of the flow

We consider flows of the form (cf. (3.28))

$$\bar{F}(t,\bar{z}) \quad = \quad \Big(F(t,z_1),\ldots,F(t,z_N)\Big) \qquad t \ge 0 \tag{3.41}$$

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

$$\frac{d}{dt}\,F(t,z) \quad = \quad g(F(t,z))\,, \qquad F(0,z)=z\,, \tag{3.42}$$

where (cf. (3.21))

$$z=(w_1,w_2,x)\in\mathbb{Z} \tag{3.43}$$

and g is a globally Lipschitz continuous vector function on $\mathbb{Z}$. One obtains (cf. (3.6))

$$\bar{g}(\bar{z}) \quad = \quad \Big(g(z_1),\ldots,g(z_N)\Big). \tag{3.44}$$

According to (3.25) and (3.44), the differential operator (3.13) takes the form

$$(\bar{D}\,\Psi)(\bar{z}) = \sum_{j=1}^{N}\sum_{k=1}^{3} g_k(z_j)\,\frac{\partial}{\partial z_{j,k}}\,\Psi(\bar{z}) \quad = \quad \sum_{j=1}^{N}(D\,\psi)(z_j)\,, \tag{3.45}$$

where

$$(D\,\psi)(z) \quad = \quad \left[g_1(z)\,\frac{\partial}{\partial w_1}+g_2(z)\,\frac{\partial}{\partial w_2}+g_3(z)\,\frac{\partial}{\partial x}\right]\psi(z)\,. \tag{3.46}$$

Consider the single particle flow

$$F(t,z)=\Big(\tilde{w}_1(t,z),\tilde{w}_2(t,z),\tilde{x}(t,z)\Big), \qquad t\ge 0\,, \qquad z\in\mathbb{Z}\,, \tag{3.47}$$

where

$$\begin{aligned}\tilde{w}_1(t,z) &= w_1\,\cos(c_{\alpha,\beta}(\varepsilon,x)\,t)-w_2\,\sin(c_{\alpha,\beta}(\varepsilon,x)\,t)\\ \tilde{w}_2(t,z) &= w_2\,\cos(c_{\alpha,\beta}(\varepsilon,x)\,t)+w_1\,\sin(c_{\alpha,\beta}(\varepsilon,x)\,t)\\ \tilde{x}(t,z) &= x\end{aligned} \tag{3.48}$$

and (cf. (2.19))

$$c_{\alpha,\beta}(\varepsilon,x) \;=\; \beta\, c_2(x) - 2\,\alpha\, c_1(\varepsilon)\,, \qquad \alpha,\beta \in [0,1]\,. \tag{3.49}$$

The weight transformation in (3.48) can be represented in the form

$$\tilde{w}_1(t,z) + i\,\tilde{w}_2(t,z) \;=\; (w_1 + i\,w_2)\, \exp(i\, c_{\alpha,\beta}(\varepsilon,x)\, t)\,. \tag{3.50}$$

One obtains

$$\frac{d}{dt}\,F(t,z) \;=\; \Big(- c_{\alpha,\beta}(\varepsilon,\tilde{x}(t,z))\,\tilde{w}_2(t,z)\,,\; c_{\alpha,\beta}(\varepsilon,\tilde{x}(t,z))\,\tilde{w}_1(t,z)\,,\; 0\Big)$$

so that (cf. (3.42))

$$g(w_1,w_2,x) \;=\; \Big(- c_{\alpha,\beta}(\varepsilon,x)\,w_2\,, c_{\alpha,\beta}(\varepsilon,x)\,w_1\,, 0\Big)$$

and the corresponding differential operator (3.46) is

$$(D\,\psi)(z) \;=\; c_{\alpha,\beta}(\varepsilon,x)\left[-w_2\,\frac{\partial}{\partial w_1} + w_1\,\frac{\partial}{\partial w_2}\right]\psi(z)\,.$$

If ψ has the form (3.26), then

$$(D\,\psi)(z) = c_{\alpha,\beta}(\varepsilon,x)\,[-w_2\,\varphi_1(x) + w_1\,\varphi_2(x)] = c_{\alpha,\beta}(\varepsilon,x)\,\psi(-w_2,w_1,x)\,. \tag{3.51}$$

specification of the jump kernel

We consider jump kernels of the form

$$\bar{Q}(\bar{z},d\bar{\kappa}) \;=\; \int_{\mathcal{Z}} \delta_{J(\bar{z};\bar{z}')}(d\bar{\kappa})\,Q(\bar{z},d\bar{z}')\,, \tag{3.52}$$

where the “offspring” creation kernel Q generates some $\bar{z}' \in \mathcal{Z}$ and the mapping

$$J:\; \mathcal{Z}\times\mathcal{Z} \to \mathcal{Z} \tag{3.53}$$

transforms $\bar{z}$ and $\bar{z}'$ into the new state $\bar{\kappa}$. The standard example of a jump transformation is

$$J(\bar{z};\bar{z}') \;=\; (z_1,\ldots,z_N,z_1',\ldots,z_{N'}')\,, \tag{3.54}$$

which simply adds the offspring to the system. According to (3.45), (3.52) and the property

$$\Psi(J(\bar{z};\bar{z}')) \;=\; \Psi(\bar{z}) + \Psi(\bar{z}')\,, \tag{3.55}$$

the extended generator (3.12) takes the form

$$(A\,\Psi)(\bar{z}) \;=\; \sum_{j=1}^{N}(D\,\psi)(z_j) + \int_{\mathcal{Z}} \Psi(\bar{z}')\,Q(\bar{z},d\bar{z}')\,. \tag{3.56}$$

Consider offspring creation kernels Q of the form (cf. (2.19))

$$Q(\bar{z}, d\bar{z}') = (1-\beta) \sum_{j=1}^{N} |c_2(x_j)| \, \delta_{(-w_{2,j} \operatorname{sign} V(x_j), w_{1,j} \operatorname{sign} V(x_j), x_j)}(d\bar{z}') + Q_1(\bar{z}, d\bar{z}') \,, \tag{3.57}$$

where $\bar{z} \in \mathcal{Z}$ (cf. (3.28)) and the kernel Q_1 generates some $\bar{z}' \in \mathcal{Z}$. Since functions of the form (3.26) satisfy

$$\psi(c\, w_1, c\, w_2, x) = c\, \psi(w_1, w_2, x) \qquad \forall\, c \in \mathbb{R}\,, \tag{3.58}$$

it follows from (3.49), (3.51) and (3.56) that

$$\begin{aligned}
(A\,\Psi)(\bar{z}) = &\sum_{j=1}^{N} \Big[\beta\, c_2(x_j) - 2\,\alpha\, c_1(\varepsilon)\Big]\, \psi(-w_{2,j}, w_{1,j}, x_j) + \\
&(1-\beta) \sum_{j=1}^{N} c_2(x_j)\, \psi(-w_{2,j}, w_{1,j}, x_j) + \int_{\mathcal{Z}} \Psi(\bar{z}')\, Q_1(\bar{z}, d\bar{z}') \\
= \;&\sum_{j=1}^{N} \Big[c_2(x_j) - 2\,\alpha\, c_1(\varepsilon)\Big]\, \psi(-w_{2,j}, w_{1,j}, x_j) + \int_{\mathcal{Z}} \Psi(\bar{z}')\, Q_1(\bar{z}, d\bar{z}')\,.
\end{aligned} \tag{3.59}$$

Lemma 3.3 *Consider the flow $\bar{F}$ defined in (3.41), (3.47)-(3.49) and jump kernels $\bar{Q}$ of the form (3.52), with the jump transformation (3.54) and offspring creation kernels (3.57). Assume that*

- *V satisfies (2.26);*
- *$\bar{Z}(0)$ satisfies (2.10) and*

$$\mathbb{P}(\bar{Z}(0) \in \mathcal{Z}_\varepsilon) \;=\; 1\,, \qquad \text{where} \quad \mathcal{Z}_\varepsilon = \cup_{N=1}^{\infty} \left(\mathbb{R}^2 \times \mathbb{R}_\varepsilon\right)^N ; \tag{3.60}$$

- *Q_1 is such that*

$$Q_1(\bar{z}, \mathcal{Z}) \;=\; Q_1(\bar{z}, \mathcal{Z}_\varepsilon) \qquad \forall\, \bar{z} \in \mathcal{Z}_\varepsilon \tag{3.61}$$

and the following conditions are fulfilled, for any $\bar{z} \in \mathcal{Z}$ (cf. (3.28)):

(1)

$$\begin{aligned}
\int_{\mathcal{Z}} \Psi(\bar{z}')\, Q_1(\bar{z}, d\bar{z}') = c_1(\varepsilon) \sum_{j=1}^{N} \Big(&\psi(-w_{2,j}, w_{1,j}, x_j - \varepsilon) + \\
&\psi(-w_{2,j}, w_{1,j}, x_j + \varepsilon) + 2\,(1-\alpha)\, \psi(w_{2,j}, -w_{1,j}, x_j)\Big),
\end{aligned} \tag{3.62}$$

for any Ψ of the form (3.25), (3.26);

(2)

$$Q_1(\bar{F}(t, \bar{z}), \mathcal{Z}) \;=\; Q_1(\bar{z}, \mathcal{Z}) \qquad \forall\, t \geq 0\,; \tag{3.63}$$

(3)

$$(1-\beta)\sum_{j=1}^{N}|c_2(x_j)|+Q_1(\bar{z},\mathcal{Z}) \quad\leq\quad H(\bar{z})\,, \tag{3.64}$$

for some function H such that

$$\mathbb{P}_{\bar{z}}\Big(H(\zeta_l)\leq H(\zeta_{l-1})+K \quad \forall\, l\geq 1\Big)=1\,, \qquad \text{for some } K>0\,, \tag{3.65}$$

where $\zeta_1\,,\zeta_2\,,\ldots$ is the embedded Markov chain for the pure jump process with the jump kernel $\bar{Q}$ and the initial state $\zeta_0=\bar{z}$;

(4)

$$\int_{\mathcal{Z}} N'\,Q_1(\bar{z},d\bar{z}') \quad\leq\quad C_1\,N\,, \qquad \text{for some} \quad C_1>0\,; \tag{3.66}$$

(5)

$$Q_1(\bar{z},\mathcal{Z}) \quad=\quad Q_1(\bar{z},\mathcal{Z}(\bar{z}))\,, \tag{3.67}$$

where

$$\mathcal{Z}(\bar{z}) \quad=\quad \Big\{\bar{z}'\in\mathcal{Z}\;:\;\max_{k=1,\ldots,N'}|w_k'|\leq\max_{j=1,\ldots,N}|w_j|\Big\} \tag{3.68}$$

and

$$w_k'=w_{1,k}'+i\,w_{2,k}'\,, \qquad w_j=w_{1,j}+i\,w_{2,j}\,. \tag{3.69}$$

Then the assumptions (i)–(iii) of Corollary 3.2 are fulfilled.

Proof. Assumption (iii) is a consequence of (3.60) and (3.61). Assumption (ii) follows from (3.58), (3.59) and (3.62). Thus, it remains to check conditions (3.7)-(3.11), (3.15), (3.16) and (3.18).

According to (3.52) and (3.57), the intensity (3.4) takes the form

$$\bar{\lambda}(\bar{z})=(1-\beta)\sum_{j=1}^{N}|c_2(x_j)|+Q_1(\bar{z},\mathcal{Z})\,. \tag{3.70}$$

It follows from (3.63) and (3.70) that

$$\bar{\lambda}(\bar{F}(t,\bar{z})) \quad=\quad \bar{\lambda}(\bar{z}) \qquad \forall\, t\geq 0\,. \tag{3.71}$$

Thus, condition (3.7) is fulfilled. According to (3.52), condition (3.8) takes the form

$$Q(\bar{z},\{\bar{z}'\in\mathcal{Z}\,:\;J(\bar{z};\bar{z}')=\bar{z}\})=0$$

and is fulfilled for any Q (cf. (3.2) and (3.54)). Condition (3.9) is a consequence of the regularity of the corresponding pure jump process (with zero flow). Indeed, according to (3.71), the distribution (3.3) of the waiting time until the next jump, and thus the distribution of the number of jumps, do not depend on the flow. According to (3.64), (3.65) and (3.70), one obtains

$$\mathbb{P}_{\bar{z}}\Big(\bar{\lambda}(\zeta_l) \le H(\bar{z}) + l\,K \quad \forall\, l = 0,1,2,\dots\Big) \;=\; 1 \qquad \forall\, \bar{z} \in \mathcal{Z}\,.$$

Thus, regularity of the pure jump process follows from the criterion (cf., e.g., [2, p.337])

$$\mathbb{P}_{\bar{z}}\left(\sum_{l=0}^{\infty} \frac{1}{\bar{\lambda}(\zeta_l)} = \infty\right) \;=\; 1 \qquad \forall\, \bar{z} \in \mathcal{Z}\,. \tag{3.72}$$

In the following, let Ψ be any function of the form (3.25), (3.26). Condition (3.10) is satisfied, since (cf. (3.41), (3.47), (3.48))

$$t \to \tilde{w}_1(t,z)\,\varphi_1(x) + \tilde{w}_2(t,z)\,\varphi_2(x) \quad \text{is absolutely continuous.} \tag{3.73}$$

Conditions (3.11), (3.15), (3.16) and (3.18) will be treated simultaneously. The proof is divided into three steps. First some sufficient conditions in terms of the total particle weight in the system are derived. Then an upper bound for the number of particles in the system is found. Finally, the various estimates are appropriately combined.

Step 1: Note that

$$|\Psi(\bar{z})| \;\le\; W(\bar{z})\Big(\|\varphi_1\|_\infty + \|\varphi_2\|_\infty\Big) \qquad \forall\, \bar{z} \in \mathcal{Z}\,, \tag{3.74}$$

where $\|.\|_\infty$ denotes the sup-norm and (cf. (3.28), (3.69))

$$W(\bar{z}) \;=\; \sum_{j=1}^{N} |w_j|\,. \tag{3.75}$$

It follows from (3.5) and (3.52) that

$$\bar{Z}(T_k)) \;=\; J(\bar{Z}(T_k-);\bar{z}'(k)) \qquad \forall\, k = 1,2,\dots\,, \tag{3.76}$$

where $\bar{z}'(k)$ denotes the offspring created at jump time T_k. According to (3.55), (3.74) and (3.76), one obtains

$$\sum_{k:\,T_k\le t}\Big|\Psi(\bar{Z}(T_k)) - \Psi(\bar{Z}(T_k-))\Big| = \sum_{k:\,T_k\le t}\Big|\Psi(\bar{z}'(k))\Big| \le \tag{3.77}$$
$$\Big(\|\varphi_1\|_\infty + \|\varphi_2\|_\infty\Big)\sum_{k:\,T_k\le t} W(\bar{z}'(k)) \le \Big(\|\varphi_1\|_\infty + \|\varphi_2\|_\infty\Big) W(\bar{Z}(t)) \qquad \forall\, t>0\,.$$

Note that each particle created at some jump time $T_k \le t$ belongs to the system (3.20) at time t, and the norm of its weight remains constant (cf. (3.50)). According to (3.77), condition (3.11) (with $\sigma_l = l$) is fulfilled provided that

$$\mathbb{E}_{\bar{z}} \sum_{j=1}^{N(t)} |w_j(t)| \;<\; \infty \qquad \forall\, t>0\,, \quad \bar{z} \in \mathcal{Z}\,. \tag{3.78}$$

It follows from (3.27) that

$$|(A\,\Psi)(\bar z)| \;\le\; C\,W(\bar z) \qquad \forall\, \bar z \in \mathcal{Z}\,, \tag{3.79}$$

where

$$C := \sup_{x\in\mathbb{R}_\varepsilon} \Big(|\varphi_1(x)| + |\varphi_2(x)|\Big)\Big(|c_2(x)| + 4\,c_1(\varepsilon)\Big) \;<\; \infty\,,$$

since φ_1, φ_2 have bounded support. The expression $W(\bar Z(t))$ is almost surely increasing with respect to t. Thus, conditions (3.15) and (3.16) are consequences of (3.74) and (3.79), respectively, provided that (3.78) is fulfilled. Finally, condition (3.18) follows from (3.74) provided that

$$\mathbb{E} \sum_{j=1}^{N(t)} |w_j(t)| \;<\; \infty \qquad \forall\, t > 0\,. \tag{3.80}$$

Step 2: First we prove that the Dynkin formula (3.17) holds for the functions

$$G_c(\bar z) \;=\; \min(N, c)\,, \qquad c > 0\,.$$

Condition (3.10) is fulfilled, since G_c does not depend on the flow. Condition (3.11) (with $\sigma_l = l$) follows from the boundedness of G_c and (3.9). Thus, $G_c \in \mathcal{D}(A)$ and (cf. (3.12), (3.45), (3.52))

$$(A\,G_c)(\bar z) \;=\; \int_{\mathcal{Z}} [G_c(J(\bar z; \bar z')) - G_c(\bar z)]\, Q(\bar z, d\bar z')\,. \tag{3.81}$$

Note that

$$0 \le G_c(J(\bar z; \bar z')) - G_c(\bar z) = \min(N + N', c) - \min(N, c) \le N'\, 1_{[0,c]}(N)\,. \tag{3.82}$$

One obtains (cf. (3.57))

$$\int_{\mathcal{Z}} N'\, Q(\bar z, d\bar z') \;=\; (1-\beta) \sum_{j=1}^{N} |c_2(x_j)| + \int_{\mathcal{Z}} N'\, Q_1(\bar z, d\bar z')\,. \tag{3.83}$$

According to (2.26), (2.19), (3.66) and (3.81)-(3.83), one obtains

$$0 \le (A\,G_c)(\bar z) \;\le\; 1_{[0,c]}(N)\, C_2\, N \le C_2\, G_c(\bar z)\,, \tag{3.84}$$

where $C_2 = \frac{q}{\hbar} V_{\max} + C_1$. Condition (3.16) is a consequence of (3.84) and condition (3.15), which follows from the boundedness of G_c . Thus, (3.17) holds with $\Psi = G_c$. It follows from (3.17) and (3.84) that

$$\begin{aligned}
\mathbb{E}_{\bar z}\, G_c(\bar Z(t)) \;&=\; G_c(\bar z) + \mathbb{E}_{\bar z} \int_0^t (A\,G_c)(\bar Z(s))\, ds \\
&\le\; G_c(\bar z) + C_2 \int_0^t (\mathbb{E}_{\bar z}\, G_c)(\bar Z(s))\, ds
\end{aligned}$$

and, according to Gronwall's inequality,

$$\mathbb{E}_{\bar{z}}\, G_c(\bar{Z}(t)) \quad \le \quad G_c(\bar{z}) \, \exp(C_2\, t) \qquad \forall\, t \ge 0\,, \quad \bar{z} \in \mathcal{Z}\,. \tag{3.85}$$

If $c \to \infty$, then $G_c(\bar{z}) \nearrow G(\bar{z}) = N$ so that (3.85) implies

$$\mathbb{E}_{\bar{z}}\, N(t) \quad \le \quad N\, \exp(C_2\, t) \qquad \forall\, t \ge 0\,, \quad \bar{z} \in \mathcal{Z}\,. \tag{3.86}$$

Step 3: According to (3.41), (3.47)-(3.50) and (3.57), (3.67), (3.68), one obtains

$$\max_{j=1,\dots,N(t)} |w_j(t)| \quad \le \quad \max_{j=1,\dots,N(0)} |w_j(0)| \qquad \forall\, t > 0\,. \tag{3.87}$$

It follows from (3.86) and (3.87) that

$$\mathbb{E}_{\bar{z}} \sum_{j=1}^{N(t)} |w_j(t)| \quad \le \quad \max_{j=1,\dots,N} |w_j|\; \mathbb{E}_{\bar{z}} N(t) \le \exp(C_2\, t)\, N \max_{j=1,\dots,N} |w_j|\,, \tag{3.88}$$

which implies condition (3.78). Finally, condition (3.80) is a consequence of (3.88) and assumption (2.10). ■

Next we consider several examples of kernels (3.57), for which the assumptions of Lemma 3.3 are fulfilled. Let $\bar{z} \in \mathcal{Z}$ (cf. (3.28)) be an arbitrary state. Define the offspring sets (cf. (3.43))

$$\begin{aligned} S_\alpha(z) \quad &= \quad \Big((-w_2, w_1, x-\varepsilon), (-w_2, w_1, x+\varepsilon), ((1-\alpha)\, w_2, -(1-\alpha)\, w_1, x), \\ &\qquad\qquad ((1-\alpha)\, w_2, -(1-\alpha)\, w_1, x)\Big), \qquad \alpha < 1\,, \\ S_1(z) \quad &= \quad \Big((-w_2, w_1, x-\varepsilon), (-w_2, w_1, x+\varepsilon)\Big), \end{aligned} \tag{3.89}$$

and

$$S_{\text{all}}(\bar{z}) = \Big(S_\alpha(z_j)\,, \quad j = 1, \dots, N\Big). \tag{3.90}$$

- According to

$$Q_1(\bar{z}, d\bar{z}') = c_1(\varepsilon) \times \tag{3.91}$$
$$\sum_{j=1}^{N} \Big(\delta_{(-w_{2,j}, w_{1,j}, x_j-\varepsilon)}(d\bar{z}') + \delta_{(-w_{2,j}, w_{1,j}, x_j+\varepsilon)}(d\bar{z}') + 2\,(1-\alpha)\, \delta_{(w_{2,j}, -w_{1,j}, x_j)}(d\bar{z}')\Big),$$

exactly one particle is created. One obtains

$$\int_{\mathcal{Z}} N'\, Q_1(\bar{z}, d\bar{z}') = Q_1(\bar{z}, \mathcal{Z}) = 2\,(2-\alpha)\, c_1(\varepsilon)\, N\,. \tag{3.92}$$

- According to

$$Q_1(\bar{z}, d\bar{z}') \quad = \quad c_1(\varepsilon) \sum_{j=1}^{N} \delta_{S_\alpha(z_j)}(d\bar{z}')\,, \tag{3.93}$$

up to four particles are created. One obtains

$$\int_{\mathcal{Z}} N'\, Q_1(\bar{z}, d\bar{z}') \le 4\, Q_1(\bar{z}, \mathcal{Z}) = 4\, c_1(\varepsilon)\, N\,. \tag{3.94}$$

- According to

$$Q_1(\bar z, d\bar z') \;=\; c_1(\varepsilon)\,\delta_{S_{\mathrm{all}}(\bar z)}(d\bar z')\,, \tag{3.95}$$

up to $4N$ particles are created. One obtains

$$\int_{\mathcal{Z}} N'\,Q_1(\bar z, d\bar z') \le 4\,N\,Q_1(\bar z, \mathcal{Z}) = 4\,N\,c_1(\varepsilon)\,. \tag{3.96}$$

Denote the set of indices of those particles in $\bar z$, which are located in x, by

$$\tilde{\mathbb{N}}(x,\bar z) \;=\; \Big\{j = 1,\dots,N \,:\, x_j = x\Big\}, \qquad x \in \mathbb{R}_\varepsilon\,,$$

and the set of positions occupied by particles in $\bar z$ by

$$\mathbb{R}_\varepsilon(\bar z) \;=\; \Big\{x \in \mathbb{R}_\varepsilon \,:\, \tilde{\mathbb{N}}(x,\bar z) \neq \emptyset\Big\}.$$

- Consider

$$\begin{aligned} &Q_1(\bar z, d\bar z') = \\ &\quad c_1(\varepsilon) \sum_{x\in\mathbb{R}_\varepsilon(\bar z)} \Big(\delta_{S^-(x,\bar z)}(d\bar z') + \delta_{S^+(x,\bar z)}(d\bar z') + 2\,(1-\alpha)\,\delta_{S^0(x,\bar z)}(d\bar z')\Big), \end{aligned} \tag{3.97}$$

where

$$\begin{aligned} S^-(x,\bar z) &= \Big((-w_{2,j}, w_{1,j}, x_j - \varepsilon)\,,\quad j \in \tilde{\mathbb{N}}(x,\bar z)\Big),\\ S^+(x,\bar z) &= \Big((-w_{2,j}, w_{1,j}, x_j + \varepsilon)\,,\quad j \in \tilde{\mathbb{N}}(x,\bar z)\Big),\\ S^0(x,\bar z) &= \Big((w_{2,j}, -w_{1,j}, x_j)\,,\quad j \in \tilde{\mathbb{N}}(x,\bar z)\Big). \end{aligned}$$

One obtains

$$\int_{\mathcal{Z}} N'\,Q_1(\bar z, d\bar z') = 2\,(1-\alpha)\,c_1(\varepsilon) \sum_{x\in\mathbb{R}_\varepsilon(\bar z)} \#\,\tilde{\mathbb{N}}(x,\bar z) = 2\,(1-\alpha)\,c_1(\varepsilon)\,N \tag{3.98}$$

and

$$Q_1(\bar z, \mathcal{Z}) \;=\; 2\,(2-\alpha)\,c_1(\varepsilon)\,\#\,\mathbb{R}_\varepsilon(\bar z)\,, \tag{3.99}$$

where the symbol $\#$ denotes the number of elements in a set.

- Consider

$$Q_1(\bar z, d\bar z') \;=\; c_1(\varepsilon) \sum_{x\in\mathbb{R}_\varepsilon(\bar z)} \delta_{S_\alpha(x,\bar z)}(d\bar z')\,, \tag{3.100}$$

where (cf. (3.89))

$$S_\alpha(x,\bar z) = \Big(S_\alpha(z_j)\,,\quad j \in \tilde{\mathbb{N}}(x,\bar z)\Big).$$

One obtains

$$\int_{\mathcal{Z}} N'\, Q_1(\bar z, d\bar z') \le 4\, c_1(\varepsilon) \sum_{x\in\mathbb{R}_\varepsilon(\bar z)} \#\,\tilde{\mathbb{N}}(x,\bar z) = 4\, c_1(\varepsilon)\, N \tag{3.101}$$

and

$$Q_1(\bar z, \mathcal{Z}) \quad = \quad c_1(\varepsilon)\,\#\,\mathbb{R}_\varepsilon(\bar z)\,. \tag{3.102}$$

In the above examples, all created particles belong to the set (3.90) so that conditions (3.61) and (3.67) are fulfilled. Condition (3.62) is easily checked using (3.58). Conditions (3.63) and (3.66) are consequences of (3.92), (3.94), (3.96), (3.98), (3.99), (3.101) and (3.102). It remains to check conditions (3.64) and (3.65).

In examples (3.91) and (3.93), the number of created particles is bounded by $K = 1$ and $K = 4$, respectively. Thus, condition (3.65) is fulfilled with the function $H(\bar z) = N$. Condition (3.64) is a consequence of (3.92) and (3.94), respectively, provided that assumption (2.26) is satisfied.

In example (3.95), the number of created particles is unbounded. If $\beta = 1$, then conditions (3.64) and (3.65) are fulfilled with the function $H(\bar z) = c_1(\varepsilon)$, according to (3.96). In this case, (3.90) is the set of *all* possible offspring of $\bar z$. Since the jump intensity is bounded, regularity follows directly from (3.72).

In examples (3.97) and (3.100), both the number of created particles and the jump intensity are unbounded. If $\beta = 1$, then condition (3.64) is fulfilled with the function

$$H(\bar z) \quad = \quad 4\, c_1(\varepsilon)\Big(\max \mathbb{R}_\varepsilon(\bar z) - \min \mathbb{R}_\varepsilon(\bar z)\Big), \tag{3.103}$$

according to (3.99) and (3.102), respectively. The function (3.103) satisfies condition (3.65) with $K = 2$.

Finally, Theorem 2.1 and its modifications are consequences of Lemma 3.3 and the examples considered above. In particular,

- the basic model (2.6)-(2.8)

  corresponds to example (3.91) with $\alpha = \beta = 1$.

  The model with particle cancellation corresponds to example (3.97) with $\alpha = \beta = 1$.

- the double-offspring model (2.20)-(2.22)

  corresponds to example (3.93) with $\alpha = \beta = 1$.

  The model with particle cancellation corresponds to example (3.100) with $\alpha = \beta = 1$.

- the multi-offspring model

  corresponds to example (3.95) with $\alpha = \beta = 1$.

  The model with particle cancellation is equivalent.

- the single-offspring models (2.23)-(2.25)

  correspond to example (3.91).

The waiting time parameters in (2.6), (2.20) and (2.23) as well as the form of the offspring weights in (2.8), (2.22) and (2.25) are determined by the kernel (3.57) with various Q_1 . Note that $-w_2 + i\,w_1 = i\,(w_1 + i\,w_2)$. The weight transformations (2.7), (2.21) and (2.24) follow from (3.50).

The modifications with particle cancellation are treated by considering auxiliary models without cancellation, in which all particles at the same position create offspring simultaneously. These auxiliary models are equivalent to the original models (with particle cancellation) in the sense that the functionals considered in Theorem 2.1, which just combine the weights in a given position, are the same in both models.

4 Comments

A class of probabilistic models for the Schrödinger equation has been introduced. This class generalizes the "random cloud model" from [17]. By using variable particle weights, the assumption concerning the boundedness of the potential V has been avoided. Moreover, the introduction of variable particle weights considerably reduces the number of jumps in the stochastic models. This makes the approach more attractive for numerical applications, compared to the original model with constant particle weights. The models were constructed for the spatially discretized one-dimensional Schrödinger equation. The generalization to a discrete multidimensional position space is straightforward. An extension to the case with a time dependent potential $V(t,x)$ should not be too difficult.

The random cloud models provide an approximate solution of the Schrödinger equation (1.1), when first taking the expectation and then letting the grid size ε go to zero. However, the issue concerning the behaviour of the stochastic models for vanishing grid size seems to be rather delicate. These models are, in a certain sense, analogous to the random walk models for the heat flow equation, which can be obtained from the Schrödinger equation by formally considering an "imaginary time". The random walk models converge to the Wiener process when $\varepsilon \to 0$. If the corresponding limits of the random cloud models exist, they will be complex-valued random fields with a rather irregular time evolution.

Extensive comments concerning the physical interpretation of the random cloud models were given in [17, Sect. 4.3] (from the perspective of a non-specialist in quantum mechanics). Some of the conceptual problems of quantum mechanics have been discussed recently in [7]. The point of view that "fields" are primary objects compared to "particles" is close in spirit to the approach via random cloud models, which might be considered as random fields.

The proof of the main result is based on the Dynkin formula for piecewise deterministic Markov processes. This class of processes has attracted increasing attention in recent years (see [1] for an overview). The application of the general theory to the class of random cloud models with variable weights required considerable effort. The main challenge was in the fact that both the jump intensity and the functional on the state space are unbounded. This issue needed a careful treatment of various conditions provided by the general theory. In the proof many different models are treated simultaneously. However, putting the generality in the formulation of Theorem 2.1 would have made the main ideas less transparent.

References

[1] R. AZAIS, J.-B. BARDET, A. GÉNADOT, N. KRELL, AND P.-A. ZITT, *Piecewise deterministic Markov process – recent results*, ESAIM: Proc., 44 (2014), pp. 276–290.

[2] L. BREIMAN, *Probability*, Addison-Wesley Publishing Company, Reading, Mass., 1968.

[3] R. COURANT, K. FRIEDRICHS, AND H. LEWY, *Über die partiellen Differenzengleichungen der mathematischen Physik*, Math. Ann., 100 (1928), pp. 32–74.

[4] M. H. A. DAVIS, *Markov Models and Optimization*, Chapman & Hall, London, 1993.

[5] R. P. FEYNMAN, *Space-time approach to non-relativistic quantum mechanics*, Rev. Modern Physics, 20 (1948), pp. 367–387.

[6] ——, *The concept of probability in quantum mechanics*, in Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability, 1950, Berkeley and Los Angeles, 1951, University of California Press, pp. 533–541.

[7] A. HOBSON, *There are no particles, there are only fields*, American Journal of Physics, 81 (2013), pp. 211–223.

[8] M. KAC, *On distributions of certain Wiener functionals*, Trans. Amer. Math. Soc., 65 (1949), pp. 1–13.

[9] ——, *Foundations of kinetic theory*, in Third Berkeley Symposium on Mathematical Statistics and Probability Theory, vol. 3, Berkeley and Los Angeles, 1956, University of California Press, pp. 171–197.

[10] A. KOLMOGOROFF, *Über die analytischen Methoden in der Wahrscheinlichkeitsrechnung*, Math. Ann., 104 (1931), pp. 415–458.

[11] M. A. LEONTOVICH, *Basic equations of the kinetic theory of gases from the point of view of the theory of random processes*, Zhurnal Ehksper. Teoret. Fiziki, 5 (1935), pp. 211–231. In Russian.

[12] G. N. MILSTEIN AND M. V. TRETYAKOV, *Stochastic Numerics for Mathematical Physics*, Springer-Verlag, Berlin, 2004.

[13] S. RJASANOW AND W. WAGNER, *Stochastic Numerics for the Boltzmann Equation*, Springer, Berlin, 2005.

[14] E. SCHRÖDINGER, *Quantisierung als Eigenwertproblem (Erste Mitteilung)*, Ann. d. Phys., 79 (1926), pp. 361–376.

[15] ——, *Quantisierung als Eigenwertproblem (Vierte Mitteilung)*, Ann. d. Phys., 81 (1926), pp. 109–139.

[16] W. WAGNER, *Stochastic models in kinetic theory*, Phys. Fluids, 23 (2011), pp. 030602(1–14).

[17] ———, *A random cloud model for the Schrödinger equation*, Kinetic and Related Models, 7 (2014), pp. 361–379.