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A random walk model for the Schrödinger equation

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Abstract

A random walk model for the spatially discretized time-dependent Schrödinger equation is constructed. The model consists of a class of piecewise deterministic Markov processes. The states of the processes are characterized by a position and a complex-valued weight. Jumps occur both on the spatial grid and in the space of weights. Between the jumps, the weights change according to deterministic rules. The main result is that certain functionals of the processes satisfy the Schrödinger equation.

Contents

1 Introduction

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

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

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) describes the time evolution of the complex-valued wave-function Φ , which represents the quantum state of the electron. It was established by Erwin Schrödinger in 1926 [8].

The probabilistic approach to quantum mechanics goes back to Feynman [5]: "A probability amplitude is associated with an entire motion of a particle as a function of time, rather than simply with a position of the particle at a particular time." Influenced by Feynman's ideas, Kac [6] introduced integration on the space of trajectories of the Wiener process [12]. The Feynman-Kac formula provides a connection between the solution of a partial differential equation and an infinite-dimensional integral. Namely, the function

$$u(t,x) \;=\; \mathbb{E}\left[\exp\left(\int_0^t c(W_x(s))\,ds\right)u_0(W_x(t))\right] \tag{1.2}$$

solves the equation

$$\frac{\partial}{\partial t}\,u(t,x) \;=\; \frac{1}{2}\,\frac{\partial^2}{\partial x^2}\,u(t,x) + c(x)\,u(t,x)\,, \tag{1.3}$$

with initial condition $u(0,x) = u_0(x)$, where c is a bounded continuous function, W_x is the Wiener process starting at x , and $\mathbb{E}$ denotes mathematical expectation (see, e.g., [9, p.56]).

This paper is concerned with the construction of a random walk model for the spatially discretized Schrödinger equation of the form

$$\frac{\partial}{\partial t}\,\Phi^{(\varepsilon)}(t,x) \;=\; \frac{i\,\hbar}{2m}\,\Delta_x^{(\varepsilon)}\,\Phi^{(\varepsilon)}(t,x) + \frac{i\,q}{\hbar}\,V(x)\,\Phi^{(\varepsilon)}(t,x) \tag{1.4}$$

where $t > 0\,,\ x \in \mathbb{R}_\varepsilon$ and

$$\mathbb{R}_\varepsilon = \Big\{\varepsilon\,j\,,\quad j = \ldots,-1,0,1,\ldots\Big\} \qquad \varepsilon > 0\,. \tag{1.5}$$

The discrete Laplacian

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

is defined for functions f on $\mathbb{R}_\varepsilon$. The model consists of a class of piecewise deterministic Markov processes (cf. [4]) depending on several parameters. The states of the processes are characterized by a position and a complex-valued weight. Jumps occur both on the spatial grid and in the space of weights. Between the jumps, the weights change according to deterministic rules. The main result is that, under suitable assumptions on the model parameters, certain functionals of the processes satisfy the Schrödinger equation (1.4).

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

2 Result

The result will be obtained for an equation that covers equation (1.4) as well as a discretized version of equation (1.3). Let

$$\kappa = \kappa_1 + i\,\kappa_2 \tag{2.1}$$

be a complex-valued constant. Consider the equation

$$\frac{\partial}{\partial t} f(t,x) = \kappa \Big[c_1(\varepsilon)\Big(f(t,x+\varepsilon) - 2\,f(t,x) + f(t,x-\varepsilon)\Big) + c_2(x)\,f(t,x)\Big], \tag{2.2}$$

where $t > 0\,,\ x \in \mathbb{R}_\varepsilon$ (cf. (1.5)) and c_1, c_2 are real-valued functions. The initial condition is

$$f(0,x) \quad = \quad f_0(x)\,, \tag{2.3}$$

where f_0 is a complex-valued function such that

$$\|f_0\| := \sum_{x\in\mathbb{R}_\varepsilon} |f_0(x)| \quad < \quad \infty\,. \tag{2.4}$$

Equation (2.2) takes the form (1.4) for the choices

$$\kappa = i\,, \qquad c_1(\varepsilon) = \frac{\hbar}{2m\,\varepsilon^2} \qquad \text{and} \qquad c_2(x) = \frac{q}{\hbar}\,V(x)\,. \tag{2.5}$$

Introduce a piecewise deterministic Markov process (cf. [4])

$$\Big(w(t), x(t)\Big) \qquad t \ge 0\,, \tag{2.6}$$

where $w(t) \in \mathbb{C}$ is a complex-valued weight and $x(t) \in \mathbb{R}_\varepsilon$ is a position. The time evolution of the process is determined by a flow F, a strictly positive measurable jump intensity λ, and a transition kernel p, as follows:

- Starting at state

  $$(w, x) \in \mathbb{C} \times \mathbb{R}_\varepsilon\,,$$

  the process performs a deterministic motion according to F.

- The random waiting time τ until the next jump satisfies

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

  where $\mathbb{P}$ is the probability measure.

- Then the process jumps into a new state

  $$(w', x') \in \mathbb{C} \times \mathbb{R}_\varepsilon\,,$$

  which is distributed according to

  $$p(F(\tau,w,x), dw', dx')\,.$$

The flow has the form

$$F(t,w,x) = \Big(\tilde{w}(t,w,x), \tilde{x}(t,w,x)\Big), \qquad t \geq 0\,, \tag{2.7}$$

where

$$\tilde{w}(t,w,x) \;=\; w\,\exp(\kappa\, c_2(x)\, t) \tag{2.8}$$

is a weight transformation and

$$\tilde{x}(t,w,x) \;=\; x\,. \tag{2.9}$$

The transition kernel has the form

$$\begin{aligned} p(w,x,dw',dx') = p_+(w,x)\,\delta_{w_+(w,x),x+\varepsilon}(dw',dx') + \\ p_-(w,x)\,\delta_{w_-(w,x),x-\varepsilon}(dw',dx') + p_0(w,x)\,\delta_{w_0(w,x),x}(dw',dx')\,, \end{aligned} \tag{2.10}$$

where p_+, p_-, p_0 are non-negative real-valued functions such that

$$p_+(w,x) + p_-(w,x) + p_0(w,x) \;=\; 1\,, \tag{2.11}$$

and w_+, w_-, w_0 are complex-valued functions. According to (2.10), the jump is

$$(w,x) \;\Rightarrow\; \begin{cases} (w_+(w,x), x+\varepsilon)\,, & \text{with probability } p_+(w,x)\,, \\ (w_-(w,x), x-\varepsilon)\,, & \text{with probability } p_-(w,x)\,, \\ (w_0(w,x), x)\,, & \text{with probability } p_0(w,x)\,. \end{cases} \tag{2.12}$$

Theorem 2.1 *Assume (cf. (2.1))*

$$\kappa_1\, c_2(x) \;\leq\; C \qquad \forall\, x \in \mathbb{R}_\varepsilon\,, \qquad \textit{for some} \quad C > 0\,. \tag{2.13}$$

Let the jump parameters be such that

$$\lambda(w,x) \;\leq\; C\,, \tag{2.14}$$

$$|w_+(w,x)| + |w_-(w,x)| + |w_0(w,x)| \;\leq\; C\,|w| \tag{2.15}$$

and

$$\begin{aligned} p_+(w,x)\,w_+(w,x) = p_-(w,x)\,w_-(w,x) = \frac{c_1(\varepsilon)}{\lambda(w,x)}\,\kappa\, w\,, \\ p_0(w,x)\,w_0(w,x) = w - \frac{2\,c_1(\varepsilon)}{\lambda(w,x)}\,\kappa\, w \qquad \forall\,(w,x) \in \mathbb{C}\times\mathbb{R}_\varepsilon\,. \end{aligned} \tag{2.16}$$

Assume that the initial state satisfies

$$\mathbb{E}\,|w(0)| \;<\; \infty\,. \tag{2.17}$$

Then the function

$$f(t,x) \;=\; \mathbb{E}\Big(w(t)\,\delta_{x(t)}(\{x\})\Big) \tag{2.18}$$

satisfies equation (2.2), with initial condition (2.3) and

$$f_0(x) \;=\; \mathbb{E}\Big(w(0)\,\delta_{x(0)}(\{x\})\Big). \tag{2.19}$$

Remark 2.2 *Assumption (2.16) implies the conservation property*

$$\int\int w'\,p(w,x,dw',dx') = \\ w_+(w,x)\,p_+(w,x) + w_-(w,x)\,p_-(w,x) + w_0(w,x)\,p_0(w,x) = w\,.$$

Remark 2.3 *Assumption (2.17) implies that the function (2.19) satisfies (2.4). This follows from the estimate*

$$\sum_{x\in\mathbb{R}_\varepsilon} |f_0(x)| \le \sum_{x\in\mathbb{R}_\varepsilon} \mathbb{E}\Big(\delta_{x(0)}(\{x\})\,|w(0)|\Big) = \mathbb{E}\,|w(0)|\,.$$

On the other hand, if some function f_0 satisfies (2.4), then the initial state of the process (2.6) can be chosen in such a way that conditions (2.17) and (2.19) hold. A particular choice is the following: Generate $x(0)$ according to the density

$$\frac{|f_0(x)|}{\|f_0\|} \qquad x\in\mathbb{R}_\varepsilon$$

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

$$w(0) \;=\; \|f_0\|\,\frac{f_0(x)}{|f_0(x)|}\,.$$

Indeed, (2.17) follows from

$$\mathbb{E}\,|w(0)| = \sum_{x\in\mathbb{R}_\varepsilon} \mathbb{E}(|w(0)|\,|\,x(0)=x)\,\mathbb{P}(x(0)=x) = \sum_{x\in\mathbb{R}_\varepsilon} |f_0(x)|\,,$$

while (2.19) is a consequence of

$$\mathbb{E}\Big(w(0)\,\delta_{x(0)}(\{x\})\Big) = \mathbb{E}(w(0)\,|\,x(0)=x)\,\mathbb{P}(x(0)=x) = f_0(x)\,.$$

Example 2.4 *Consider the case*

$$\kappa_1 = 0\,,$$

which covers equation (1.4) (cf. (2.5)). Condition (2.13) is fulfilled for any function c_2 . Condition (2.16) implies

$$\int\int |w'|\,p(w,x,dw',dx') = |w|\left(\frac{2\,c_1(\varepsilon)\,\kappa_2}{\lambda(w,x)} + \sqrt{1+\frac{4\,c_1(\varepsilon)^2\,\kappa_2^2}{\lambda(w,x)^2}}\right) \quad > \quad |w|$$

and

$$|w_0(w,x)| = \frac{1}{p_0(w,x)}\,\sqrt{1+\frac{4\,c_1(\varepsilon)^2\,\kappa_2^2}{\lambda(w,x)^2}}\;|w| \quad > \quad |w|\,.$$

Thus, the norm of the weight is unbounded. If

$$p_+(w,x) = p_-(w,x) = p_0(w,x) = \frac{1}{3}$$

and

$$\lambda(w,x) > 3\,|c_1(\varepsilon)\,\kappa_2|\,,$$

then condition (2.16) implies

$$|w_+(w,x)| = |w_-(w,x)| \quad < \quad |w|\,.$$

Thus, the norm of the weight goes up and down, depending on the jumps on the spatial grid.

Example 2.5 *Consider the case*

$$\kappa_1\,c_1(\varepsilon) > 0\,, \qquad \kappa_2 = 0\,,$$

which covers a discretized version of equation (1.3). If

$$\lambda(w,x) \quad \geq \quad 2\,\kappa_1\,c_1(\varepsilon)\,,$$

then condition (2.16) is satisfied for the parameters

$$w_+(w,x) = w_-(w,x) = w_0(w,x) = w$$

and

$$p_+(w,x) = p_-(w,x) = \frac{\kappa_1\,c_1(\varepsilon)}{\lambda(w,x)}\,, \qquad p_0(w,x) = 1 - \frac{2\,\kappa_1\,c_1(\varepsilon)}{\lambda(w,x)}\,.$$

The standard random walk is obtained for

$$\lambda(w,x) \quad = \quad 2\,\kappa_1\,c_1(\varepsilon)\,.$$

3 Proof

Theorem 2.1 is proved using the theory of piecewise deterministic processes (cf. [4]). First, some facts from the theory are recalled. Then, it is shown that the basic assumptions of the theory follow from the conditions in the Theorem. Finally, equation (2.2) is derived from Dynkin's formula.

For various complex-valued quantities we will use the notations

$$f = f_1 + i\,f_2\,, \qquad w = w_1 + i\,w_2 \tag{3.1}$$

and, e.g.,

$$\begin{aligned} \kappa\,w \quad &= \quad (\kappa_1 + i\,\kappa_2)\,(w_1 + i\,w_2) = \kappa_1\,w_1 - \kappa_2\,w_2 + i\,(\kappa_2\,w_1 + \kappa_1\,w_2) \\ &= \quad (\kappa\,w)_1 + i\,(\kappa\,w)_2\,. \end{aligned} \tag{3.2}$$

3.1 General theory

The process (2.6) is represented in the form

$$Z(t) \quad = \quad \Big(w_1(t), w_2(t), x(t)\Big) \qquad t \geq 0\,. \tag{3.3}$$

Let

$$z = (w_1, w_2, x) \in \mathbb{Z}\,, \qquad \text{where} \quad \mathbb{Z} = \mathbb{R} \times \mathbb{R} \times \mathbb{R}_\varepsilon\,. \tag{3.4}$$

The flow (2.7) takes the form

$$F(t,z) = \Big(\tilde{w}_1(t,z), \tilde{w}_2(t,z), \tilde{x}(t,z)\Big) \qquad t \geq 0\,, \tag{3.5}$$

where $\tilde{x}(t,z) = x$ and

$$\begin{aligned} \tilde{w}_1(t,z) &= \exp(\kappa_1\, c_2(x)\, t)\Big[w_1\, \cos(\kappa_2\, c_2(x)\, t) - w_2\, \sin(\kappa_2\, c_2(x)\, t)\Big] \\ \tilde{w}_2(t,z) &= \exp(\kappa_1\, c_2(x)\, t)\Big[w_2\, \cos(\kappa_2\, c_2(x)\, t) + w_1\, \sin(\kappa_2\, c_2(x)\, t)\Big]. \end{aligned}$$

Indeed, the weight transformation (2.8) satisfies

$$\begin{aligned} \tilde{w}(t,z) &= \tilde{w}_1(t,z) + i\, \tilde{w}_2(t,z) = (w_1 + i\, w_2)\, \exp((\kappa_1 + i\, \kappa_2)\, c_2(x)\, t) \\ &= (w_1 + i\, w_2)\, \exp(\kappa_1\, c_2(x)\, t)\Big[\cos(\kappa_2\, c_2(x)\, t) + i\, \sin(\kappa_2\, c_2(x)\, t)\Big]. \end{aligned}$$

regularity

It has to be checked that the “standard” conditions are satisfied, for any $z \in \mathbb{Z}$:

- the intensity λ is such that

$$t \to \lambda(F(t,z)) \quad \text{is integrable on finite intervals;} \tag{3.6}$$

- the process is regular, i.e.,

$$\mathbb{E}_z\, \#\{l : T_l \leq t\} < \infty \qquad \forall\, t > 0\,, \tag{3.7}$$

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

extended generator

According to [4, Theorem 26.14], the domain $\mathcal{D}(\mathcal{A})$ of the extended generator of the process (3.3) consists of all measurable functions ψ such that, for any $z \in \mathbb{Z}$,

$$t \to \psi(F(t,z)) \quad \text{is absolutely continuous} \tag{3.8}$$

and

$$\mathbb{E}_z \left(\sum_{l:\, T_l \le \sigma_n} \Big| \psi(Z(T_l)) - \psi(Z(T_l-)) \Big| \right) < \infty \qquad \forall\, n = 1, 2, \ldots\,, \tag{3.9}$$

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

$$\begin{aligned}(\mathcal{A}\,\psi)(w_1, w_2, x) \;&=\; \lambda(z)\Big(p_+(z)\Big[\psi(w_{+,1}(z), w_{+,2}(z), x+\varepsilon) - \psi(z)\Big] + \\ &\quad p_-(z)\Big[\psi(w_{-,1}(z), w_{-,2}(z), x-\varepsilon) - \psi(z)\Big] + \\ &\quad p_0(z)\Big[\psi(w_{0,1}(z), w_{0,2}(z), x) - \psi(z)\Big]\Big) + (D\,\psi)(z)\,,\end{aligned} \tag{3.10}$$

where

$$(D\,\psi)(z) \;=\; c_2(x)\left[(\kappa_1\, w_1 - \kappa_2\, w_2)\,\frac{\partial}{\partial w_1} + (\kappa_2\, w_1 + \kappa_1\, w_2)\,\frac{\partial}{\partial w_2}\right]\psi(z)\,. \tag{3.11}$$

Indeed, the weight transformation (2.8) satisfies

$$\begin{aligned}\frac{d}{dt}\,\tilde{w}(t,z) \;&=\; w\,\kappa\, c_2(x)\, \exp(\kappa\, c_2(x)\, t) = \kappa\, c_2(x)\,\tilde{w}(t,z) \\ &=\; c_2(x)\,\Big[(\kappa_1\,\tilde{w}_1(t,z) - \kappa_2\,\tilde{w}_2(t,z)) + i\,(\kappa_2\,\tilde{w}_1(t,z) + \kappa_1\,\tilde{w}_2(t,z))\Big],\end{aligned}$$

which implies

$$\frac{d}{dt}\,\tilde{w}_1(t,z) \;=\; c_2(x)\,\Big[\kappa_1\,\tilde{w}_1(t,z) - \kappa_2\,\tilde{w}_2(t,z)\Big]$$

and

$$\frac{d}{dt}\,\tilde{w}_2(t,z) \;=\; c_2(x)\,\Big[\kappa_2\,\tilde{w}_1(t,z) + \kappa_1\,\tilde{w}_2(t,z)\Big].$$

One obtains (cf. (3.5))

$$\frac{d}{dt}\,F(t,z) \;=\; g(\tilde{w}_1(t,z), \tilde{w}_2(t,z), \tilde{x}(t,z))\,,$$

where

$$g(w_1, w_2, x) \;=\; \Big(c_2(x)\,(\kappa_1\, w_1 - \kappa_2\, w_2)\,,\; c_2(x)\,(\kappa_2\, w_1 + \kappa_1\, w_2)\,,\; 0\Big),$$

which leads to (3.11).

Dynkin's formula

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

$$M_t(\psi) = \psi(Z(t)) - \psi(z) - \int_0^t (\mathcal{A}\,\psi)(Z(s))\,ds\,, \qquad t \ge 0\,, \tag{3.12}$$

is a local martingale. If

$$\mathbb{E}_z \sup_{s\in[0,t]} |\psi(Z(s))| < \infty \qquad \forall\, t>0\,, \quad z\in\mathbb{Z}\,, \tag{3.13}$$

and

$$\mathbb{E}_z \sup_{s\in[0,t]} |(\mathcal{A}\,\psi)(Z(s))| < \infty \qquad \forall\, t>0\,, \quad z\in\mathbb{Z}\,, \tag{3.14}$$

then the process (3.12) is a martingale and one obtains the Dynkin formula

$$\mathbb{E}_z\,\psi(Z(t)) \;=\; \psi(z)+\mathbb{E}_z\int_0^t (\mathcal{A}\,\psi)(Z(s))\,ds \qquad \forall\, t>0\,, \quad z\in\mathbb{Z}\,. \tag{3.15}$$

If

$$\mathbb{E}\,|\psi(Z(t))| < \infty \qquad \forall\, t\geq 0\,, \tag{3.16}$$

then (3.15) implies

$$\mathbb{E}\,\psi(Z(t)) \;=\; \mathbb{E}\,\psi(Z(0))+\mathbb{E}\int_0^t (\mathcal{A}\,\psi)(Z(s))\,ds\,. \tag{3.17}$$

3.2 Application

We use the assumptions of Theorem 2.1 in order to check conditions (3.6), (3.7) (related to the regularity of the process), (3.8), (3.9) (characterizing the domain of the extended generator) and (3.13), (3.14), (3.16) (assuring the validity of the Dynkin formula).

Consider functions on $\mathbb{Z}$ (cf. (3.4)) of the form

$$\psi(z) \;=\; w_1\,\varphi_1(x)+w_2\,\varphi_2(x)\,, \tag{3.18}$$

where φ_1 and φ_2 are bounded. Note that

$$|\psi(z)| \;\leq\; |w|\Big(\|\varphi_1\|_\infty+\|\varphi_2\|_\infty\Big), \tag{3.19}$$

where $\|.\|_\infty$ denotes the sup-norm. According to (2.11), assumption (2.16), (3.10) and (3.11), one obtains (cf. (3.1), (3.2))

$$\begin{aligned}
(\mathcal{A}\,\psi)(z) = {} & \lambda(z)\,p_+(z)\Big[w_{+,1}(z)\,\varphi_1(x+\varepsilon)+w_{+,2}(z)\,\varphi_2(x+\varepsilon)\Big]+\\
& \lambda(z)\,p_-(z)\Big[w_{-,1}(z)\,\varphi_1(x-\varepsilon)+w_{-,2}(z)\,\varphi_2(x-\varepsilon)\Big]+\\
& \lambda(z)\,p_0(z)\Big[w_{0,1}(z)\,\varphi_1(x)+w_{0,2}(z)\,\varphi_2(x)\Big]-\lambda(z)\Big[w_1\,\varphi_1(x)+w_2\,\varphi_2(x)\Big]+\\
& c_2(x)\,\Big[(\kappa_1\,w_1-\kappa_2\,w_2)\,\varphi_1(x)+(\kappa_2\,w_1+\kappa_1\,w_2)\,\varphi_2(x)\Big]\\
= {} & c_1(\varepsilon)\Big[(\kappa\,w)_1\,\varphi_1(x+\varepsilon)+(\kappa\,w)_2\,\varphi_2(x+\varepsilon)\Big]+ \qquad (3.20)\\
& c_1(\varepsilon)\Big[(\kappa\,w)_1\,\varphi_1(x-\varepsilon)+(\kappa\,w)_2\,\varphi_2(x-\varepsilon)\Big]-\\
& 2\,c_1(\varepsilon)\Big[(\kappa\,w)_1\,\varphi_1(x)+(\kappa\,w)_2\,\varphi_2(x)\Big]+c_2(x)\Big[(\kappa\,w)_1\,\varphi_1(x)+(\kappa\,w)_2\,\varphi_2(x)\Big]
\end{aligned}$$

and

$$|(\mathcal{A}\,\psi)(z)| \le |w|\,|\kappa| \left[4\,c_1(\varepsilon)\Big(\|\varphi_1\|_\infty + \|\varphi_2\|_\infty\Big) + \|c_2\,\varphi_1\|_\infty + \|c_2\,\varphi_2\|_\infty\right]. \qquad (3.21)$$

The right-hand side of (3.21) is finite if φ_1 and φ_2 have compact support, or, if c_2 is bounded.

Conditions (3.6) and (3.7) follow from assumption (2.14). Condition (3.8) is fulfilled, according to (2.8) and (2.9). The remaining conditions will follow from rather rough estimates for the weight components of the process (3.3).

According to (2.8) and assumption (2.13), one obtains

$$|\tilde{w}(t,w,x)| \quad\le\quad |w|\,\exp(C\,t)$$

so that (cf. (3.7))

$$|w(s)| \quad\le\quad |w(T_{l-1})|\,\exp(C\,(s-T_{l-1})) \qquad \forall\, s\in[T_{l-1},T_l)\,, \qquad l=1,2,\ldots. \qquad (3.22)$$

According to (2.10) (cf. (2.12)) and assumption (2.15), one obtains

$$|w(T_l)| \quad\le\quad C\,|w(T_l-)| \qquad \forall\, l=1,2,\ldots. \qquad (3.23)$$

It follows from (3.22) and (3.23) that

$$\begin{aligned} |w(s)| &\le C\,|w(T_{l-1}-)|\,\exp(C\,(s-T_{l-1})) \\ &\le C^{l-1}\,|w(0)|\,\exp(C\,s) \qquad \forall\, s\in[T_{l-1},T_l)\,, \qquad l=1,2,\ldots, \end{aligned}$$

and

$$\sup_{s\in[0,t]} |w(s)| \quad\le\quad C^{\alpha(t)}\,|w(0)|\,\exp(C\,t) \qquad \forall\, t\ge 0\,, \qquad (3.24)$$

where

$$\alpha(t) \quad=\quad \max\Big\{l=0,1,2,\ldots\,:\, T_l\le t\Big\} \qquad (3.25)$$

is the number of jumps before t. Moreover, (3.24) implies

$$\mathbb{E}_z \sum_{l:\,T_l\le n} \Big(|w(T_l)|+|w(T_l-)|\Big) \quad\le\quad 2\,|w|\,\exp(C\,n)\;\mathbb{E}_z\Big(\alpha(n)\,C^{\alpha(n)}\Big). \qquad (3.26)$$

According to assumption (2.14), one obtains

$$\mathbb{E}_z\,\alpha(t)\,C^{\alpha(t)} \quad\le\quad \sum_{k=0}^{\infty} k\,C^k\,\frac{(C\,t)^k}{k!}\,\exp(-C\,t) \le C^2\,t\,\exp(C^2\,t)\,. \qquad (3.27)$$

Condition (3.9) (with $\sigma_n = n$) follows from (3.19), (3.26) and (3.27).

Condition (3.13) is a consequence of (3.19), (3.24) and (3.27).

Condition (3.14) follows from (3.21), (3.24) and (3.27).

Condition (3.16) is a consequence of (3.19), (3.24), (3.27) and assumption (2.17).

3.3 Derivation of the equation

According to (2.18), one obtains (cf. (3.1))

$$f_j(t,x) \;=\; \mathbb{E}\Big(w_j(t)\,\delta_{x(t)}(\{x\})\Big), \qquad j=1,2\,,$$

and

$$\sum_x \varphi(x)\, f_j(t,x) \;=\; \mathbb{E}\Big[w_j(t)\,\varphi(x(t))\Big], \tag{3.28}$$

for any bounded function φ . It follows from (3.28) that (cf. (3.18))

$$\mathbb{E}\,\psi(w_1(t),w_2(t),x(t)) \;=\; \sum_x \Big[\varphi_1(x)\, f_1(t,x) + \varphi_2(x)\, f_2(t,x)\Big] \tag{3.29}$$

and (cf. (3.2))

$$\mathbb{E}\Big[(\kappa\, w(t))_j\, \varphi(x(t))\Big] \;=\; \sum_x \varphi(x)\,(\kappa\, f(t,x))_j\,. \tag{3.30}$$

According to (3.20) and (3.30), one obtains

$$\begin{aligned}
&\mathbb{E}\,(\mathcal{A}\,\psi)(w_1(t),w_2(t),x(t)) = \\
&\quad c_1(\varepsilon)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x+\varepsilon) + (\kappa\, f(t,x))_2\,\varphi_2(x+\varepsilon)\Big] + \\
&\quad c_1(\varepsilon)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x-\varepsilon) + (\kappa\, f(t,x))_2\,\varphi_2(x-\varepsilon)\Big] - \\
&\quad 2\,c_1(\varepsilon)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x) + (\kappa\, f(t,x))_2\,\varphi_2(x)\Big] + \\
&\quad c_2(x)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x) + (\kappa\, f(t,x))_2\,\varphi_2(x)\Big].
\end{aligned} \tag{3.31}$$

Dynkin's formula (3.17) implies that the quantity $\mathbb{E}\,\psi(Z(t))$ is continuous, for any function ψ of the form (3.18), where φ_1 and φ_2 have compact support. In particular, one obtains

$$\lim_{t\to 0}\mathbb{E}\,\psi(w_1(t),w_2(t),x(t)) \;=\; \mathbb{E}\,\psi(w_1(0),w_2(0),x(0))\,. \tag{3.32}$$

According to (3.20), the quantity $\mathbb{E}\,(\mathcal{A}\,\psi)(Z(t))$ is also continuous so that (3.17) implies

$$\frac{d}{dt}\,\mathbb{E}\,\psi(w_1(t),w_2(t),x(t)) \;=\; \mathbb{E}\,(\mathcal{A}\,\psi)(w_1(t),w_2(t),x(t))\,. \tag{3.33}$$

Equation (2.2) will be derived from (3.33). The initial condition (2.3) follows from (3.32).

According to (3.29) and (3.31), equation (3.33) takes the form

$$\frac{d}{dt}\sum_x \Big[\varphi_1(x)\, f_1(t,x) + \varphi_2(x)\, f_2(t,x)\Big] =$$

$$
\begin{aligned}
&c_1(\varepsilon)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x+\varepsilon)+(\kappa\, f(t,x))_2\,\varphi_2(x+\varepsilon)\Big]+\\
&c_1(\varepsilon)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x-\varepsilon)+(\kappa\, f(t,x))_2\,\varphi_2(x-\varepsilon)\Big]-\\
&2\,c_1(\varepsilon)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x)+(\kappa\, f(t,x))_2\,\varphi_2(x)\Big]+\\
&c_2(x)\sum_x \Big[(\kappa\, f(t,x))_1\,\varphi_1(x)+(\kappa\, f(t,x))_2\,\varphi_2(x)\Big]. \qquad (3.34)
\end{aligned}
$$

By choosing appropriate test functions one obtains from (3.34) the equations

$$
\begin{aligned}
\frac{\partial}{\partial t}\, f_1(t,x) &= c_2(x)\,(\kappa\, f(t,x))_1 + \qquad (3.35)\\
&\quad c_1(\varepsilon)\Big[(\kappa\, f(t,x-\varepsilon))_1+(\kappa\, f(t,x+\varepsilon))_1-2\,(\kappa\, f(t,x))_1\Big]
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial}{\partial t}\, f_2(t,x) &= c_2(x)\,(\kappa\, f(t,x))_2 + \qquad (3.36)\\
&\quad c_1(\varepsilon)\Big[(\kappa\, f(t,x-\varepsilon))_2+(\kappa\, f(t,x+\varepsilon))_2-2\,(\kappa\, f(t,x))_2\Big]\,.
\end{aligned}
$$

Equation (2.2) is equivalent to the system of equations

$$
\begin{aligned}
&\frac{\partial}{\partial t}\, f_1(t,x) = \\
&\quad \kappa_1\,\Big[c_1(\varepsilon)\Big(f_1(t,x+\varepsilon)-2\,f_1(t,x)+f_1(t,x-\varepsilon)\Big)+c_2(x)\,f_1(t,x)\Big]-\\
&\quad \kappa_2\,\Big[c_1(\varepsilon)\Big(f_2(t,x+\varepsilon)-2\,f_2(t,x)+f_2(t,x-\varepsilon)\Big)+c_2(x)\,f_2(t,x)\Big]
\end{aligned}
$$

and

$$
\begin{aligned}
&\frac{\partial}{\partial t}\, f_2(t,x) = \\
&\quad \kappa_1\,\Big[c_1(\varepsilon)\Big(f_2(t,x+\varepsilon)-2\,f_2(t,x)+f_2(t,x-\varepsilon)\Big)+c_2(x)\,f_2(t,x)\Big]+\\
&\quad \kappa_2\,\Big[c_1(\varepsilon)\Big(f_1(t,x+\varepsilon)-2\,f_1(t,x)+f_1(t,x-\varepsilon)\Big)+c_2(x)\,f_1(t,x)\Big],
\end{aligned}
$$

which takes the form (3.35), (3.36).

4 Comments

Here we provide some general remarks on the random walk model (2.6) and discuss connections with related topics.

relation to Feynman integrals

An elementary introduction to Feynman integrals is given in [7]. A function K is called Green's function, fundamental solution, or propagator, if it provides a solution to equation (1.1) via

$$\Phi(t,x) \quad = \quad \int_{-\infty}^{\infty} K(t,y,x)\, \Phi_0(y)\, dy\,, \tag{4.1}$$

where

$$\Phi_0(x) \quad = \quad \lim_{t\to 0} \Phi(t,x)$$

is the initial value. Very roughly, Feynman's idea [5] was the representation

$$K(t,y,x) \quad = \quad \int_{\text{paths}\, z\,:\, z(0)=y\,,\, z(t)=x} \exp\left(\frac{i}{\hbar}\, S[z]\right) \text{"}Dz\text{"}\,,$$

where

$$S[z] \quad = \quad \int_0^t \left\{\frac{m}{2}\, z'(s)^2 + q\, V(z(s))\right\} ds$$

and "Dz" is a symbolic integration (superposition of probability amplitudes). When discretizing the interval $[0,t]$, replacing the derivative by a difference quotient, and introducing an appropriate normalizing factor, one obtains

$$K(t,y,x) = \lim_{N\to\infty} \left(\frac{m}{2\pi\, i\, \hbar\, \Delta t}\right)^{N/2} \times \tag{4.2}$$
$$\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \exp\left(\frac{i}{\hbar} \sum_{j=1}^{N} \left\{\frac{m\,(z_j - z_{j-1})^2}{2\,\Delta t} + q\, V(z_j)\, \Delta t\right\}\right) dz_1 \ldots dz_{N-1}\,,$$

where

$$\Delta t = \frac{t}{N}\,, \qquad z_0 = y \qquad \text{and} \qquad z_N = x\,. \tag{4.3}$$

Under appropriate regularity assumptions, a solution of the discretized equation (1.4) converges to a solution of the Schrödinger equation (1.1), as $\varepsilon \to 0$. In this case, Theorem 2.1 implies

$$\Phi(t,x) = \lim_{\varepsilon\to 0} \Phi^{(\varepsilon)}(t,x) = \lim_{\varepsilon\to 0} \mathbb{E}\, \xi^{(\varepsilon)}(t,x)\,, \tag{4.4}$$

where

$$\xi^{(\varepsilon)}(t,x) \quad = \quad w^{(\varepsilon)}(t)\, \delta_{x^{(\varepsilon)}(t)}(\{x\})\,. \tag{4.5}$$

Note that the process (2.6) depends on ε via the state space (1.5) and the jump parameters (cf. (2.16)). There is a certain analogy between the representations (4.4) and (4.1), (4.2). However, the approximation parameter ε in (4.4) refers to space discretization, while the approximation parameter N in (4.2) refers to time discretization.

relation to the Feynman-Kac formula

Kac [6] justified Feynman's approach in a specific situation, where integration is performed with respect to the Wiener measure [12]. The result can be illustrated heuristically by using "imaginary time". With

$$D = \frac{\hbar}{2m} \qquad \text{and} \qquad c(x) = \frac{q}{\hbar} V(x)\,, \tag{4.6}$$

representation (4.2) implies

$$K(-i\,t, y, x) = \lim_{N\to\infty} \left(\frac{1}{\sqrt{4\pi\, D\, \Delta t}} \right)^{N} \times \tag{4.7}$$

$$\int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp\left(\sum_{j=1}^{N} \left\{ -\frac{(z_j - z_{j-1})^2}{4\, D\, \Delta t} + c(z_j)\, \Delta t \right\} \right) dz_1 \dots dz_{N-1}$$

$$= \lim_{N\to\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \left(\prod_{j=1}^{N} p(\Delta t, z_{j-1}, z_j) \right) \exp\left(\sum_{j=1}^{N} c(z_j)\, \Delta t \right) dz_1 \dots dz_{N-1}\,,$$

where

$$p(t, y, x) \quad = \quad \frac{1}{\sqrt{4\pi\, D\, t}} \exp\left(-\frac{(x-y)^2}{4\, D\, t} \right). \tag{4.8}$$

Note that (4.7) can be obtained using Trotter-Kato theory, which extends Lie's product formula (for non-commutative matrices) to certain unbounded operators and implies

$$e^{(A+B)\,t} \quad = \quad \lim_{N\to\infty} \left(e^{A\Delta t}\, e^{B\Delta t} \right)^{N}\,.$$

Indeed, function (4.8) is the fundamental solution of the diffusion equation

$$\frac{\partial}{\partial t} u(t, x) \quad = \quad A_x\, u(t, x) := D\, \Delta_x u(t, x)\,, \tag{4.9}$$

while the function

$$b(t, y, x) \quad = \quad \delta(x-y)\, \exp(t\, c(x))$$

is the fundamental solution of the equation

$$\frac{\partial}{\partial t} u(t, x) \quad = \quad B_x\, u(t, x) := c(x)\, u(t, x)\,.$$

Function (4.8) is the transition density of the Wiener process (with standard deviation $2D$) and satisfies the Chapman-Kolmogorov equation (semigroup property). Thus, if $V = 0$ (free electron), then (4.7) implies

$$K(-i\,t, y, x) = \lim_{N\to\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \left(\prod_{j=1}^{N} p(\Delta t, z_{j-1}, z_j) \right) dz_1 \dots dz_{N-1} = p(t, x, y)$$

so that

$$K(t,y,x) = p(i\,t,y,x)\,.$$

If F is some functional of the Wiener trajectory W , then one obtains

$$\begin{aligned} p(t,y,x)\,\mathbb{E}_{t,y,x}\,F[W] &= \int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty} dz_1\ldots dz_{N-1}\left(\prod_{j=1}^{N} p(\Delta t, z_{j-1}, z_j)\right)\times \\ & \qquad \mathbb{E}_{t,y,x}\Big(F[W]\Big|\,W(t_1)=z_1,\ldots,W(t_{N-1})=z_{N-1}\Big), \end{aligned} \tag{4.10}$$

where (cf. (4.3))

$$t_i = i\,\Delta t \qquad i = 0,1,\ldots,N\,,$$

and $\mathbb{E}_{t,y,x}$ denotes expectation conditioned on $W(0) = y$, $W(t) = x$. According to (4.10), with

$$F[W] = \exp\left(\sum_{j=1}^{N} c(W(t_j))\,\Delta t\right),$$

(4.7) takes the form

$$K(-i\,t,y,x) = p(t,y,x)\lim_{N\to\infty}\mathbb{E}_{t,y,x}\,\exp\left(\sum_{j=1}^{N} c(W(t_j))\,\Delta t\right), \tag{4.11}$$

which corresponds to a time discretization in the Feynman-Kac formula (1.2).

Theorem 2.1 provides a spatially discretized version of the Feynman-Kac formula. Indeed, consider equation (2.2) with (cf. (4.6))

$$\kappa = 1\,, \qquad c_1(\varepsilon) = \frac{D}{\varepsilon^2}\,, \qquad c_2(x) = c(x)\,,$$

and Example 2.5 with

$$\lambda(w,x) = 2\,c_1(\varepsilon)\,. \tag{4.12}$$

Let $T_1, T_2, \ldots$ be the jump times of the process (2.6), and $T_0 = 0$. Then (2.8) implies (cf. (3.25))

$$w^{(\varepsilon)}(t) = w^{(\varepsilon)}(0)\,\exp\left(\sum_{l=1}^{\alpha(t)} c(x^{(\varepsilon)}(T_{l-1}))\,(T_l - T_{l-1}) + c(x^{(\varepsilon)}(T_{\alpha(t)}))\,(t - T_{\alpha(t)})\right) \tag{4.13}$$

and (cf. (4.4), (4.5))

$$\Phi(t,x) = \lim_{\varepsilon\to 0}\mathbb{E}\left(w^{(\varepsilon)}(t)\,\delta_{x^{(\varepsilon)}(t)}(\{x\})\right). \tag{4.14}$$

Let $p^{(\varepsilon)}$ denote the transition density of the random walk $x^{(\varepsilon)}$. If $x^{(\varepsilon)}(0) = y$ and $w^{(\varepsilon)}(0) = 1$ (cf. Remark 2.3), then (4.14) takes the form

$$\begin{aligned} \Phi(t,x) &= \lim_{\varepsilon\to 0}\int \mathbb{E}\left(w^{(\varepsilon)}(t)\,\delta_{x^{(\varepsilon)}(t)}(\{x\})\,\Big|\,x^{(\varepsilon)}(t) = z\right)p^{(\varepsilon)}(t,y,z)\,dz \\ &= \lim_{\varepsilon\to 0} p^{(\varepsilon)}(t,y,x)\,\mathbb{E}\left(w^{(\varepsilon)}(t)\,\Big|\,x^{(\varepsilon)}(t) = x\right). \end{aligned} \tag{4.15}$$

remarks concerning the limiting processes

In the case of real-valued functionals (or, “imaginary time”), the limiting procedures in (4.11) ($N \to \infty$) and (4.15) ($\varepsilon \to 0$) can be performed, leading to the Wiener process. Indeed, under appropriate regularity assumptions on c , it follows from (4.11) that

$$K(-i\,t, y, x) \;\;=\;\; p(t, y, x)\; \mathbb{E}_{t,y,x}\, \exp\left(\int_0^t c(W(s))\, ds\right). \tag{4.16}$$

According to (4.16), one obtains

$$\begin{aligned} u(t, x) \;\;&=\;\; \int dy\, u_0(y)\, p(t, y, x)\; \mathbb{E}_{t,y,x}\, \exp\left(\int_0^t c(W(s))\, ds\right) \\ &=\;\; \mathbb{E}\left[u_0(W(0))\, \exp\left(\int_0^t c(W(s))\, ds\right) \Big|\, W(t) = x)\right], \end{aligned}$$

which, after a substitution of the time variable, takes the form (1.2). On the other hand, due to the random walk approximation property of the Wiener process, it follows from (4.13) and (4.15) that

$$\Phi(t, x) \;\;=\;\; p(t, y, x)\; \mathbb{E}\left[\exp\left(\int_0^t c(W(s))\, ds\right) \Big|\, W(0) = y\,,\, W(t) = x\right],$$

which is (4.16).

In the case of complex-valued functionals, the situation is much more complicated. Concerning (4.2), Feynman [5] made the remark: “There are very interesting mathematical problems involved in the attempt to avoid the subdivision and limiting processes”. Various efforts to justify and develop Feynman’s approach have created an enormous literature (see, e.g., [1]). Regarding (4.4), interesting open questions concern the existence of

$$\lim_{\varepsilon \to 0} \xi^{(\varepsilon)}(t, x)$$

and the exchangeability of the limit and the expectation. The spatial component $x^{(\varepsilon)}(t)$ makes small jumps with a large intensity (cf. (4.12)). In the limit $\varepsilon \to 0$, it should still converge to a Wiener process, which is slightly modified due to the fact that there are jumps $x \to x$. The weight component $w^{(\varepsilon)}(t)$ makes jumps, which do not vanish in the limit. This may lead to some generalized process in the spirit of “white noise”. Moreover, the spatial component and the weight component are not independent.

general remarks on the model

The random walk model (2.6) has been constructed for equation (2.2), which covers the spatially discretized versions of both the Schrödinger equation (1.1) and its real-valued modification (1.3). This emphasizes the analogy with the classical results from [3] concerning the connections between random walks and difference equations. It also provides a discrete version of the Feynman-Kac formula, which is different from that obtained via the Feynman integrals.

The proof of Theorem 2.1 is based on Dynkin's formula for piecewise deterministic Markov processes. This class of processes has attracted increasing attention in recent years (see [2] for an overview). The model (2.6) has been developed for the one-dimensional position space. The generalization to the multi-dimensional case is straightforward.

The general concept behind the model (2.6) are weighted particle systems. The positive solution (4.8) of the diffusion equation (4.9) can be approximated as

$$p(t,y,x)\,dx \quad \sim \quad \frac{1}{n}\sum_{i=1}^{n} \delta_{W_y^{(i)}(t)}(dx)\,, \tag{4.17}$$

where $W_y^{(i)}$ are independent Wiener processes starting at y . In analogy with (4.17), the complex-valued solution of the Schrödinger equation (1.1) should be approximated via

$$\Phi(t,x)\,dx \quad \sim \quad \sum_{i=1}^{n} w_i(t)\,\delta_{x_i(t)}(dx)\,.$$

More generally, vector-valued weights might be used to approximate solutions of systems of equations.

The concept of weighted particles has been implemented in the "random cloud models", which were introduced in [10] and extended in [11]. In the random cloud models, the number of particles in the system is growing, but the individual weights are bounded. In the random walk model (2.6), the number of particles remains constant, but the weights are growing. The random cloud models seem to be more appropriate for numerical purposes, since cancellation effects can be explicitly included.

It is not clear if the random walk model will be of any use for specific quantum mechanical calculations. However, it provides an alternative view on the probabilistic interpretation of the Schrödinger equation. A probabilistic representation of the solution is obtained by considering trajectories of a particle in an extended state space, instead of considering, e.g., complex-valued "probability" measures. This extended state, which includes a complex-valued weight, leads to various superposition effects and is characteristic for a "quantum" particle compared to a classical diffusive particle.

References

[1] S. A. Albeverio, R. J. Høegh-Krohn, and S. Mazzucchi, *Mathematical theory of Feynman path integrals*, vol. 523 of Lecture Notes in Mathematics, Springer-Verlag, Berlin, second ed., 2008.

[2] 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.

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

[7] J. B. KELLER AND D. W. MCLAUGHLIN, *The Feynman integral*, Amer. Math. Monthly, 82 (1975), pp. 451–465.

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

[9] S. R. S. VARADHAN, *Stochastic processes*, vol. 16 of Courant Lecture Notes in Mathematics, Courant Institute of Mathematical Sciences, New York; American Mathematical Society, Providence, RI, 2007.

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

[11] ——, *A class of probabilistic models for the Schrödinger equation*, Monte Carlo Methods Appl., 21 (2015). To appear (published online 04/24/2015).

[12] N. WIENER, *Differential-space*, J. Math. and Phys., 2 (1923), pp. 131–174.