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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.

Keywords: Schrödinger equation; Probabilistic representation; Random walk model; Piecewise deterministic Markov process

1. Introduction

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

$$i\,\hbar\,\frac{\partial}{\partial t}\,\Phi(t,x) = -\frac{\hbar^2}{2m}\,\Delta_x\,\Phi(t,x) - q\,V(x)\,\Phi(t,x), \tag{1}$$

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. Eq. (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 [15].

The probabilistic approach to quantum mechanics goes back to Feynman [4]: "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 [22]. The Feynman–Kac formula provides a connection between the solution of a partial differential equation and an infinite-dimensional integral. Namely, the function

$$u(t,x) = \mathbb{E}\left[\exp\left(\int_0^t c(W_x(s))\,ds\right) u_0(W_x(t))\right] \tag{2}$$

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solves the equation

$$\frac{\partial}{\partial t} u(t,x) = \frac{1}{2} \frac{\partial^2}{\partial x^2} u(t,x) + c(x)\, u(t,x), \tag{3}$$

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., [18, p. 56]).

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

$$\frac{\partial}{\partial t} \Phi^{(\varepsilon)}(t,x) = \frac{i\,\hbar}{2m} \Delta_x^{(\varepsilon)} \Phi^{(\varepsilon)}(t,x) + \frac{i\,q}{\hbar} V(x)\, \Phi^{(\varepsilon)}(t,x), \tag{4}$$

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

$$\mathbb{R}_\varepsilon = \Big\{ \varepsilon\, j,\ j = \cdots, -1, 0, 1, \ldots \Big\}. \tag{5}$$

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. [3]) 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 (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. Main result

Consider the equation

$$\frac{\partial}{\partial t} f(t,x) = \kappa \Big[c_1(\varepsilon) \Big(f(t,x+\varepsilon) - 2\, f(t,x) + f(t,x-\varepsilon) \Big) + c_2(x)\, f(t,x) \Big], \tag{6}$$

where $t > 0,\ x \in \mathbb{R}_\varepsilon,\ \kappa \in \mathbb{C}$ is a complex number and c_1, c_2 are real-valued functions. Eq. (6) takes the form (4) for the choices

$$\kappa = i, \qquad c_1(\varepsilon) = \frac{\hbar}{2m\,\varepsilon^2} \quad \text{and} \quad c_2(x) = \frac{q}{\hbar} V(x). \tag{7}$$

It also covers a discretized version of Eq. (3). We introduce a piecewise deterministic Markov process (cf. [3])

$$\Big(w(t), x(t) \Big) \quad t \geq 0, \tag{8}$$

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

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

  where $\mathbb{P}$ is the probability measure.
- At time τ, the process jumps into a new state $(w',x') \in \mathbb{C} \times \mathbb{R}_\varepsilon$, which is distributed according to $p(F(\tau,w,x), dw', dx')$.