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Quantum Simulation of the Fokker-Planck Equation via Schrödingerization

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Abstract. This paper studies a quantum simulation technique for solving the Fokker-Planck equation. Traditional semi-discretization methods often fail to preserve the underlying Hamiltonian dynamics and may even modify the Hamiltonian structure, particularly when incorporating boundary conditions. We address this challenge by employing the Schrödingerization method – it converts any linear partial and ordinary differential equation with non-Hermitian dynamics into systems of Schrödinger-type equations. It does so via the so-called warped phase transformation that maps the equation into one higher dimension. We explore the application in two distinct forms of the Fokker-Planck equation. For the conservation form, we show that the semi-discretization-based Schrödingerization is preferable, especially when dealing with non-periodic boundary conditions. Additionally, we analyze the Schrödingerization approach for unstable systems that possess positive eigenvalues in the real part of the coefficient matrix or differential operator. Our analysis reveals that the direct use of Schrödingerization has the same effect as a stabilization procedure. For the heat equation form, we propose a quantum simulation procedure based on the time-splitting technique, and give explicitly its corresponding quantum circuit. We discuss the relationship between operator splitting in the Schrödingerization method and its application directly to the original problem, illustrating how the Schrödingerization method accurately reproduces the time-splitting solutions at each step. Furthermore, we explore finite difference discretizations of the heat equation form using shift operators. Utilizing Fourier bases, we diagonalize the shift operators, enabling efficient simulation in the frequency space. Providing additional guidance on implementing the diag-

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onal unitary operators, we conduct a comparative analysis between diagonalizations in the Bell and the Fourier bases, and show that the former generally exhibits greater efficiency than the latter.

AMS subject classifications: 68Q12, 81P68, 68Q25, 65N22

Key words: Fokker-Planck equation, Schrödingerization, quantum simulation, shift operators, diagonal unitary operators.

1 Introduction

The Fokker-Planck equation is a fundamental evolution equation used to model various stochastic processes in statistical mechanics, plasma physics, fluid dynamics, neural networks, machine learning, and socio-economic modeling [14,16,21,34,39,41,43,44,48,49], among others. It governs the behavior of a wide class of Markov processes and is particularly important for describing systems influenced by drag forces and random forces. The linear form of the Fokker-Planck equation is given by

$$\partial_t f = \nabla\cdot(f\nabla V(x)) + \sigma\Delta f, \tag{1.1}$$

In this equation, $f = f(t,x) \geq 0$ represents the unknown density function, $V(x)$ is an external potential, and $\sigma > 0$ is a constant. The equation describes the time evolution of the probability density function of a particle's position. The first term on the right-hand side is the drift term, while the second term represents diffusion generated by white noise. It is worth noting that the Fokker-Planck equation possesses a steady-state solution given by $f = \exp(-V(x)/\sigma)$ [43]. In this context, we assume periodic boundary conditions, where $x = (x_1,\cdots,x_d) \in \Omega = (-1,1)^d$, for convenience.

A main challenge in classical numerical simulation of the Fokker-Planck equation is the curse-of-dimensionality, since it is typically high-dimensional partial differential equation (PDE) in statistical physics and machine learning, for example. In recent years there is increasing activity in developing quantum algorithms to be used on quantum computers – yet to be developed in the future – to solve PDEs [2,8,10,11,13,15,17,25,31,37,40], many of which rely upon the exponential speedup advantages in quantum linear systems of equations [2,4,9,11,12,19,47]. A strategy for crafting quantum PDE solvers involves discretizing spatial variables to yield a system of ordinary differential equations (ODEs), which can then be tackled using quantum ODE solvers [2,4,11]. Notably, if the solution operator to the resulting ODE system is a unitary system, quantum simulations can be executed with reduced time complexity compared to quantum ODE solvers or other quantum linear algebra solvers (like quantum difference methods) [2,31]. If the system is not a unitary one needs to "dilate" it to a unitary system [6,7,18,32].

In a recent work, a new, simple and generic framework coined *Schrödingerization* was introduced in [30,32] that allows quantum simulation for *all* linear PDEs and ODEs. The