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QUANTUM SIMULATION OF A CLASS OF HIGHLY-OSCILLATORY TRANSPORT EQUATIONS VIA SCHRÖDINGERISATION*

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Abstract

In this paper, we present quantum algorithms for a class of highly-oscillatory transport equations, which arise in semi-classical computation of surface hopping problems and other related non-adiabatic quantum dynamics, based on the Born-Oppenheimer approximation. Our method relies on the classical nonlinear geometric optics method, and the recently developed Schrödingerisation approach for quantum simulation of partial differential equations. The Schrödingerisation technique can transform any linear ordinary and partial differential equations into Hamiltonian systems evolving under unitary dynamics, via a warped phase transformation that maps these equations to one higher dimension. We study possible paths for better recoveries of the solution to the original problem by shifting the bad eigenvalues in the Schrödingerized system. Our method ensures the uniform error estimates independent of the wave length, thus allowing numerical accuracy, in maximum norm, even without numerically resolving the physical oscillations. Various numerical experiments are performed to demonstrate the validity of this approach.

Mathematics subject classification: 35L25, 65N35, 68Q12, 81P68.
Key words: Quantum simulation, Schrödingerisation, Highly oscillatory transport PDEs, Nonlinear geometric optics method.

1. Introduction

As the classical computer is increasingly closer to its physical limit [24], a potentially effective path to the future computing platform is quantum computing [23], which are currently under rapid development. Compared with classical methods, quantum algorithms have already been shown to have certain advantages in a number of problems [16, 18, 41]. For instance, the HHL algorithm proposed by Harrow, Hassidim and Lloyd [25] can realize exponential acceleration when solving systems of linear equations under several conditions. Such successful cases motivate one to extend the high-cost classical algorithms of important scientific problems to quantum algorithms [17, 43, 44]. In particular, quantum algorithms for solving ordinary or partial differential equations have received extensive recent attention [6, 12–14, 19, 34, 37].

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In this paper, we concentrate on a family of transport equations in which the phase oscillations depend on both time and space as follows:

$$\partial_t u + \sum_{k=1}^{d} A_k(x)\partial_{x_k} u = \frac{iE(t,x)}{\varepsilon} Du + Cu,$$
$$u(0,x) = u_0(x), \quad x \in \Omega \subset \mathbb{R}^d,$$

where $u(t,x) \in \mathbb{C}^n$, A_k and D are $n \times n$ real symmetric matrices, $C \in \mathbb{R}^{n\times n}$, E is a real scalar function. The initial function is the given initial data which may have a periodic oscillation with the phase $\beta(x)/\varepsilon$, i.e. $u_0(x) = f_0(x, \beta(x)/\varepsilon)$. A number of semi-classical models in quantum dynamics can be written in this form, such as surface hopping [11], graphene [39], quantum dynamics in periodic lattice [38], etc. Solving such systems is computationally daunting since 1) often the dimension is high ($d \gg 1$), and 2) one needs to numerically resolve the small wave lengths which are of $\mathcal{O}(\varepsilon)$ [22, 36]. While Hamiltonian simulation provides a principled approach to solving the Schrödinger formulation of such applications – for instance, via quantum algorithms designed for semi-classical Schrödinger equations [8, 26], these methods do need to use mesh sizes that depend on ε.

The nonlinear geometric optics (NGO) based method, developed in [15] for above problems, uses a nonlinear geometric optics ansatz which builds the oscillatory phase as an independent variable, and a suitably chosen initial data derived from the Chapman-Enskog expansion, guarantee that one can use mesh size and time step independent of ε. However, the curse-of-dimensionality remains the bottleneck for classical computation. This motivates us to consider quantum algorithms for this problem, which has no curse-of-dimensionality due to the use of qubits, since in general one just needs $n = \mathcal{O}(d \log N)$ qubits for d-dimensional problems, where N is the number of discretization points per dimension.

Although existing Hamiltonian simulation algorithms (e.g. quantum Magnus expansion methods [9, 21, 40, 42]) can effectively simulate many highly oscillatory systems governed by anti-Hermitian operators, the core difficulty in this case arises from the non-anti-Hermitian character of the operator, primarily due to the inclusion of the C term. Our main tool for quantum simulation is a new method called Schrödingerisation which have been recently proposed for solving general linear ordinary and partial differential equations [33, 34]. This technique can convert non-unitary dynamics (linear differential equations) to unitary dynamics (Schrödinger type equations) by a warped phase transformation that just maps the system to one higher dimension, followed by a Fourier transform. The original variable can be recovered via integration on or pointwise evaluation of the extra variable. This method works for both qubits [33, 34] and continuous-variable frameworks [29], open quantum systems with artificial boundary conditions [28], physical boundary or interface conditions [27], etc., and problems with time-dependent coefficients [3, 4, 7, 10, 20]. Other possible candidates for the problem include discretization based approaches such as linear algebra-based HHL algorithm [25], and the linear combination of Hamiltonian simulation, as outlined in [1, 2, 5], if one is interested in qubit framework, not continuous variable frameworks.

The outline of this paper is as follows. In Section 2, we give a brief review of the Schrödingerisation method. Then, based on the nonlinear geometric optics approach, we apply the Schrödingerisation algorithm together with spectral and finite difference discretisations on the equations, for one dimensional scalar equations in Section 3. We provide numerical results for problems of different settings. In Section 4, we extend the new approach to a class of PDE system which is the semi-classical approximation of surface hopping problem [11], and show the effectiveness of