COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **4**, No. 5, pp. 980-1007

Commun. Comput. Phys.
November 2008

Review Article

The Quantum Lattice Boltzmann Equation: Recent Developments†

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Received 26 February 2008; Accepted (in revised version) 25 June 2008

Available online 8 July 2008

Abstract. The derivation of the quantum lattice Boltzmann model is reviewed with special emphasis on recent developments of the model, namely, the extension to a multi-dimensional formulation and the application to the computation of the ground state of the Gross-Pitaevskii equation (GPE). Numerical results for the linear and non-linear Schrödinger equation and for the ground state solution of the GPE are also presented and validated against analytical results or other classical schemes such as Crank-Nicholson.

PACS: 02.70.-c, 03.65-w, 03.67.Lx

Key words: Quantum lattice Boltzmann, multi-dimensions, imaginary-time model, linear and non-linear Schrödinger equation, adiabatic limit.

Contents

†Dedicated to Professor Xiantu He on the occasion of his 70th birthday.
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1 Introduction

Lattice Boltzmann models (LBMs) have become a competitive numerical tool for simulating fluid flows over a wide range of complex physical problems [1–7]. LBMs were initially derived from lattice gas cellular automata (LGCA). The basic idea of LGCA is to simulate the macroscopic behavior of a fluid flow by implementing an extremely simplified model of the microscopic interactions between particles. LBMs were developed, starting from LGCA, in the attempt to overcome their major drawbacks: statistical noise, increasing complexity of the collision operator (for three dimensional problems) and high viscosity (due to small number of collisions) [1–3]. Nowadays, LBM has consolidated into a powerful alternative to more classical computational fluid dynamics models based on the discretization of the Navier-Stokes equations of continuum mechanics.

However, LBM and, in general, the lattice kinetic approach has been mostly used with classical (non-quantum) fluid. Nonetheless, with the theorization of quantum computers, some authors have extended the lattice kinetic approach to quantum mechanics [8–16]. In fact, as it was first suggested by Feynman [17], the most natural application of quantum computers would be quantum mechanics [18]. The lattice kinetic approach is very interesting in this respect, because it was shown that the so-called quantum lattice gas cellular automata (QLGCA) [11] can be used to simulate systems of nonrelativistic quantum particles with exponential speedup in the number of particles [8].

Besides their hypothetical and future application to quantum computing , these lattice kinetic methods for quantum mechanics are interesting numerical schemes, which can be implemented on classical computers retaining the usual attractive features of LGCA and LBM: simplicity, computational speed, straightforward parallel implementation.

In this paper, we will focus on the so-called quantum lattice Boltzmann (qLB) model proposed by Succi and Benzi [16,19]. The qLB model was initially derived from a formal parallel between the kinetic lattice Boltzmann equation (LBE) and the relativistic Dirac equation. It was then shown that the non-relativistic Schrödinger equation ensues from the Dirac equation under an adiabatic assumption that is formally similar to the one which takes the Boltzmann equation to the Navier-Stokes equations in kinetic theory [16].

The basic idea of the qLB model is to associate the wave functions composing the Dirac quadrispinor with the discrete distribution functions of the LBE. In one spatial dimension, this analogy is natural and the quadrispinor components can be assimilated to quantum particles of different types propagating with velocities $\pm c$ and colliding when they meet at the same space-time location. However, in multi-dimensional formulation, the analogy is no longer straightforward. This is mainly due to the fact that the Dirac streaming operator is not diagonal along all the spatial directions (i.e., Dirac matrices can not be simultaneously diagonalized). We could roughly say that, unlike classical