Journal of Computational Physics 291 (2015) 303–316

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Numerical scheme for a spatially inhomogeneous matrix-valued quantum Boltzmann equation ☆

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ARTICLE INFO

Article history:
Received 8 August 2014
Received in revised form 23 January 2015
Accepted 10 March 2015
Available online 18 March 2015

Keywords:
Quantum Boltzmann equation
Hubbard model
Fourier spectral method

ABSTRACT

We develop an efficient algorithm for a spatially inhomogeneous matrix-valued quantum Boltzmann equation derived from the Hubbard model. The distribution functions are 2×2 matrix-valued to accommodate the spin degree of freedom, and the scalar quantum Boltzmann equation is recovered as a special case when all matrices are proportional to the identity. We use Fourier discretization and fast Fourier transform to efficiently evaluate the collision kernel with spectral accuracy, and numerically investigate periodic, Dirichlet and Maxwell boundary conditions. Model simulations quantify the convergence to local and global thermal equilibrium.

1. Introduction

Boltzmann's kinetic theory is widely used to describe the dynamics of rarified gases. Immediately after the discovery of quantum mechanics, a modification of the classical Boltzmann equation to take quantum interactions into account has been proposed by Nordheim [12] (with a more systematic derivation by Peierls [13]), and by Uehling and Uhlenbeck [18,19]. With the inclusion of quantum mechanical effects into the collision operator, the quantum Boltzmann equation has many applications, e.g., for the kinetic description of Bose–Einstein condensation [15,16], spintronics and decoherence theory in quantum computing [2,14,20,22], or kinetic modeling of semiconductor devices [9].

In recent works, starting from the Hubbard model in the weak interaction limit, a matrix-valued Boltzmann equation has been derived [4–6] for the spatially homogeneous setting without advection term. To describe spatially inhomogeneous systems, one combines the Boltzmann transport equation with the collision term derived in [4]:

$$\partial_t W + v_x \partial_x W = \mathscr{C}[W] - i[\vec{B} \cdot \vec{\sigma}, W], \tag{1}$$

where the state variable W is the Wigner distribution of the spin-density matrix, $\vec{B}$ is an external magnetic field, $\vec{\sigma}$ are the Pauli matrices, and the collision term $\mathscr{C}[W]$ will be specified below in Section 2. We emphasize that while the form of the equation follows the usual quantum Boltzmann equation, the collision term is quite different (which is systematically derived from a many-body quantum mechanics model), and the matrix-valued W distinguishes the equation from the usual kinetic equations.

☆ We would like to thank Jingwei Hu, Lorenzo Pareschi and Herbert Spohn for helpful discussions. The work of J.L. was supported in part by the Alfred P. Sloan Foundation and the National Science Foundation under award DMS-1312659. C.M. would like to thank the warm hospitality of the Mathematics Department at Duke University where part of the work was done, as well as support from DFG under grant FR 1275/3-1.

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http://dx.doi.org/10.1016/j.jcp.2015.03.020
0021-9991/

The focus of this paper is devising an efficient algorithm for solving (1). Our goal in this work is twofold: First, we would like to develop a numerical scheme that systematically converges to the true solution; for that purpose, we use a spectral method in the velocity variable. The collision operator, albeit much more complicated than for the usual classical or scalar quantum Boltzmann equation, can be efficiently calculated using Carleman representation and fast Fourier transforms. Second, we want to investigate non-trivial boundary conditions, like Dirichlet and Maxwell boundary conditions, and the effect of external magnetic fields. These developments should lead to a better understanding of the physics modeled by these equations.

Kinetic equations are traditionally solved by Monte Carlo methods (also known as particle methods). In recent years, the development of efficient real space or Fourier space methods to solve Boltzmann equations has been a very active research area. In particular, the line of research initiated by [11] and further developed in [3,7] is especially relevant for our approach. The paper [11] proposed a fast algorithm for computing the Boltzmann collision kernel based on Fourier discretization, and [7] further improved the efficiency of the algorithm. The method we develop in this work for the collision operator of the matrix-valued Boltzmann equation is closely related, albeit with some differences: (a) Since we are dealing with collision terms originating from quantum mechanics, the microscopic energy is not necessarily conserved (see the effective Hamiltonian in Eq. (6) below); some new ideas are required to treat the resulting terms. (b) To evaluate double convolutions exactly using fast Fourier transforms, we use a double padding approach to avoid aliasing issues. As a result, while maintaining the spectral accuracy, the scheme also nicely respects the conservation law of the continuous equation. Further details can be found in Section 3.

A numerical algorithm for the spatially homogeneous matrix-valued Boltzmann equation in one dimension was considered before in [5,6], which calculates the collision term directly using numerical quadrature. A subsequent work by one of the authors [10] considers a lattice Boltzmann method (LBM) for the spatially inhomogeneous equation with periodic boundary conditions, which can be understood as a discrete velocity method with very few velocity grid points. Due to the small number of grid points, the accuracy of the numerical result compared to the original equation is not guaranteed. In contrast to that, the method proposed here systematically approximates the original equation as we refine the grid.

Considering the *matrix-valued* Boltzmann equation, it is useful to represent the spin-density Wigner distribution in the basis of Pauli matrices. In fact, the formulas for the collision terms are more compact in the new representation, which might be of independent interest for understanding the physics and mathematics of the equation.

The rest of the paper is organized as follows. We introduce the spatially inhomogeneous matrix-valued Boltzmann equation and its associated boundary conditions in Section 2. We will focus on the development of the fast algorithm for the collision operator in Section 3. To deal with the spatial degree of freedom, we use the finite volume method and a parallel implementation based on MPI; this is discussed in Section 4. We show some numerical results for validating the algorithm and for exploring interesting physical phenomena in Section 5. Finally we wrap up the paper with some conclusive remarks in Section 6.

2. The spatially inhomogeneous matrix-valued Boltzmann equation

The starting point for the derivation [4] of the matrix-valued Boltzmann equation is the Hubbard model with a weak pair potential λV such that $0 < \lambda \ll 1$. Consider a spin-$\frac{1}{2}$ Fermi field with annihilation operators $a_s(x)$, $x \in \mathbb{Z}^d$, $s \in \{\uparrow, \downarrow\}$, obeying the anti-commutation relations

$$\left\{a_s(x)^\dagger, a_{s'}(x')\right\} = \delta_{xx'}\delta_{ss'}, \quad \left\{a_s(x), a_{s'}(x')\right\} = 0, \quad \text{and} \quad \left\{a_s(x)^\dagger, a_{s'}(x')^\dagger\right\} = 0,$$

where $A^\dagger$ denotes the adjoint operator of A. Using the second quantization formulation, the (many-body) Hamiltonian of the Hubbard system is then given by

$$H = \sum_{x,y\in\mathbb{Z}^d} \sum_{s\in\{\uparrow,\downarrow\}} \alpha(x-y) a_s(x)^\dagger a_s(y) + \frac{1}{2} \sum_{x\in\mathbb{Z}^d} \sum_{s,s'\in\{\uparrow,\downarrow\}} \lambda V(x-y) a_s(x)^\dagger a_s(x) a_{s'}(y)^\dagger a_{s'}(y). \tag{2}$$

Here the first term on the right hand side in the Hamiltonian describes the hopping from site y to x with α the hopping amplitude, and the non-quadratic second term gives the interactions of two excitons with V the interaction potential. The grid $\mathbb{Z}^d$ must be distinguished from the spatial dimension considered below (in some sense, the grid $\mathbb{Z}^d$ is on the microscopic scale while the spatial inhomogeneity is introduced on a mesoscopic scale). In Fourier representation, the time-dependent (Heisenberg picture) field operators $\hat{a}_s(t, v)$ adhere to the initial ($t = 0$) anti-commutation relation $\{\hat{a}_s(v)^\dagger, \hat{a}_{s'}(v')\} = \delta_{ss'}\delta(v - v')$, with v, v' denoting velocity variables. As discussed in [4], the time-dependent average Wigner matrix W defined by

$$\left\langle \hat{a}_s(t, v)^\dagger \hat{a}_{s'}(t, v') \right\rangle = \delta(v - v') W_{ss'}(t, v) \tag{3}$$

will approximately satisfy a Boltzmann kinetic equation $\partial_t W = \mathscr{C}[W]$ for times up to order λ^{-2}. Here, as in the Heisenberg picture, the average $\langle\cdot\rangle$ is taken with respect to the initial state of the system. The effective Boltzmann equation is much easier to solve compared to the original quantum many-body system, which is an extremely high-dimensional problem.

Augmenting the Boltzmann equation with the usual transport term for the spatially inhomogeneous setting and including an external magnetic field $\vec{B}$, one arrives at Eq. (1), where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices: