

# The Hyperbolic Schrödinger Equation and the Quantum Lattice Boltzmann Approximation

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*To the memory of R.E. O'Malley*

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**Abstract.** The quantum lattice Boltzmann (qlB) algorithm solves the 1D Dirac equations and has been used to solve approximately the classical (i.e., non-relativistic) Schrödinger equation. We point out that the qlB method actually approximates the *hyperbolic* version of the non-relativistic Schrödinger equation, whose solution is thus obtained at the price of an additional small error. Such an error is of order of  $(\omega_c \tau)^{-1}$ , where  $\omega_c := \frac{mc^2}{\hbar}$  is the Compton frequency,  $\hbar$  being the reduced Planck constant,  $m$  the rest mass of the electrons,  $c$  the speed of light, and  $\tau$  a chosen reference time (i.e., 1 s), and hence it vanishes in the non-relativistic limit  $c \rightarrow +\infty$ . This asymptotic result comes from a singular perturbation process which does not require any boundary layer and, consequently, the approximation holds uniformly, which fact is relevant in view of numerical approximations. We also discuss this occurrence more generally, for some classes of linear singularly perturbed partial differential equations.

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## 1 Introduction

“Hyperbolic” versions of the Schrödinger equation exist in some contexts [9, 35, 38], and also emerge operating a certain transformation on the Klein-Gordon equation [10, 11]. Hyperbolic Schrödinger-like equations are strictly connected to the Dirac system, which provides a relativistic description of Quantum Mechanics. It was pointed out, e.g., in [10, 11, 23, 24] that the classical (non-relativistic) Schrödinger equation and the hyperbolic

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Schrödinger equation are related to each other by a singular perturbation, and in fact Fattorini refers more properly to this issue as to “the Schrödinger singular perturbation problem”, since the classification as “hyperbolic” should be considered only formal. In [23,24,32,33], Schrödinger singular perturbations have been considered using an abstract formulation of the corresponding initial-value problem.

The so-called quantum lattice Boltzmann (qlB) scheme, which is a quantum mechanics version of the “(Gas) Lattice Boltzmann” method [27, 29], has been adopted to solve numerically the Dirac system in a very efficient way. It was also exploited to solve numerically the non-relativistic Schrödinger equation [17, 18, 20, 26, 30]; see also the review article [19]. However, it turns out that the qlB method actually provides the solution to the hyperbolic rather than to the non-relativistic Schrödinger equation; see Section 2.4 below. Therefore, aiming at solving the latter, one can indeed solve the Dirac system but then the sought result is achieved at the price of the error made in the aforementioned singular perturbation.

In Section 2, we first review some well known results of Quantum Mechanics [21,22]. Then, we derive two coupled hyperbolic Schrödinger-like equations satisfied by the so-called fast and slow complex-valued fields, strictly related to the Dirac’s quadrispinor. In some cases, these equations decouple exactly, in some others approximately (depending on the external field’s size and nonlinearity), yielding single hyperbolic Schrödinger-like equations. We also show that, in general, one could obtain a single fourth-order equation for each of the two fields alone. In Section 2.4, we recall few facts on the qlB method. In Section 3 and Section 4, we discuss singular perturbation problems for certain classes of partial differential equations (PDEs) which do not require any boundary layer. The case of the Schrödinger singular perturbation problem can be cast in this framework, resulting in a *uniform* error of order of  $\mathcal{O}(\varepsilon)$  on the closed time-interval  $[0, T]$ , for any  $T > 0$ , being  $\varepsilon := \frac{\hbar}{2mc^2\tau} \equiv (2\omega_c\tau)^{-1}$ , where

$$\omega_c := \frac{mc^2}{\hbar} \tag{1.1}$$

is the Compton frequency,  $\hbar = \frac{h}{2\pi}$  is the reduced Planck constant ( $h$  being the Planck constant),  $m$  the rest mass of the electrons,  $c$  the speed of light, and  $\tau$  is a reference time (e.g.,  $\tau = 1s$ ; see Section 2.2 for a discussion on scales. Note that  $\omega_c \rightarrow +\infty$  and  $\varepsilon := \frac{\hbar}{2mc^2\tau} \equiv (2\omega_c\tau)^{-1} \rightarrow 0$  in the non-relativistic limit  $c \rightarrow +\infty$ . In Section 5, we discuss such an error in terms of Fourier or Fourier-Laplace transforms and then in the original  $(x, t)$  domain. Details are relegated to an Appendix. In Section 6, finally, we summarize the high points of the paper.

## 2 The hyperbolic Schrödinger equation and the quantum lattice Boltzmann approximation

In this section, we review some well known results of Quantum Mechanics [21, 22]. The hyperbolic form of the Schrödinger equation is introduced and the relation with the Dirac