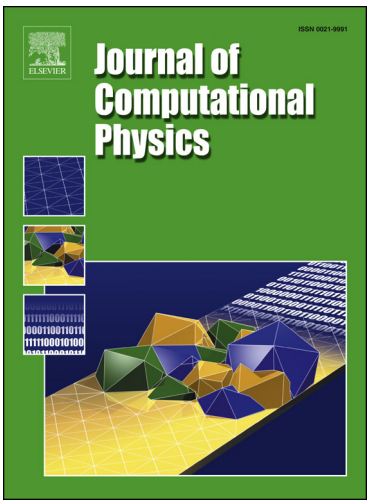
Accepted Manuscript



Single-cone finite difference scheme for the (2+1)D Dirac von Neumann equation

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PII: S0021-9991(17)30545-4
DOI: http://dx.doi.org/10.1016/j.jcp.2017.07.037
Reference: YJCPH 7484

To appear in: *Journal of Computational Physics*

Received date: 25 August 2016
Revised date: 18 July 2017
Accepted date: 19 July 2017

Please cite this article in press as: W. Pötz, M. Schreilechner, Single-cone finite difference scheme for the (2+1)D Dirac von Neumann equation, *J. Comput. Phys.* (2017), http://dx.doi.org/10.1016/j.jcp.2017.07.037

Single-cone finite difference scheme for the (2+1)D Dirac von Neumann equation

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Abstract

An explicit finite difference scheme is presented for the von Neumann equation for (2+1)D Dirac fermions. It is founded upon a staggered space-time grid which ensures a single-cone energy dispersion and performs the time-derivative in one sweep using a three-step leap-frog procedure. It enables a space-time-resolved numerical treatment of the mixed-state dynamics of Dirac fermions within the effective single-particle density matrix formalism. Energy-momentum dispersion, stability and convergence properties are derived. Elementary numerical tests to demonstrate stability properties use parameters which pertain to topological insulator surface states. A method for the simulation of charge injection from an electric contact is presented and tested numerically. Potential extensions of the scheme to a Dirac-Lindblad equation, real-space-time Green's function formulations, and higher-order finite-difference schemes are discussed.

Keywords: Dirac equation, von Neumann equation, finite-difference scheme, staggered grid, fermion doubling, topological insulator

1. Introduction - preliminaries and definitions

1.1. The Dirac equation and numerical schemes

In the context of graphene and, more recently, topological insulator surface states, the Dirac equation has received renewed interest within the physics community. Introduced by P. A. M. Dirac in 1928, the (3+1)D Dirac equation has been the standard model for relativistic spin-1/2 particles. It is a key ingredient to the Standard Model of elementary particle physics[1–5]. In condensed matter and atomic physics its non-relativistic limit provides the spin-orbit interaction, which is instrumental to an understanding of atomic spectra and represents the foundation for the entire field of spintronics[6]. In electronic structure calculations the full Dirac equation has been used to describe inner shell electrons[7, 8]. The (1+1)D and (2+1)D versions of the Dirac equation allow a two-dimensional representation of the Clifford algebra. In the early days of quantum physics they were used for model studies, however, condensed matter physics has recently delivered spectacular physical realizations of (2+1)D Dirac fermions as the low energy electronic excitations in graphene and topological insulators (TIs)[9–14].

With the interest in graphene and TIs as components of electronic and spintronic devices efficient schemes for the numerical solution of the (2+1)D Dirac equation have become desirable. Numerical approaches for solving the Dirac equation have taken several approaches. For investigations of relativistic electrons in atomic physics, a (2+1)D fast Fourier transformation (FFT) split-operator code was used [15, 16]. In such an approach, FFT between the space and momentum representation is used to compute the Dirac propagator. The computational effort generally scales in $\mathcal{O}(N \ln N)$, where N is the number of grid-points. An efficient code using operator splitting in real space was introduced for the (3+1)D case [17]. It leads to

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