Commun. Comput. Phys.
doi: 10.4208/cicp.110914.281014a

Vol. **17**, No. 3, pp. 850-866
March 2015

The Split-Operator Technique for the Study of Spinorial Wavepacket Dynamics

A. Chaves[1,*], G. A. Farias[1], F. M. Peeters[1,2] and R. Ferreira[1,3]

[1] *Departamento de Física, Universidade Federal do Ceará, Caixa Postal 6030, Campus do Pici, 60455-900 Fortaleza, Ceará, Brazil.*
[2] *Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium.*
[3] *Laboratoire Pierre Aigrain, Ecole Normale Superieure, 24 Rue Lhomond, F-75005, Paris, France.*

Received 11 September 2014; Accepted (in revised version) 28 October 2014

Abstract. The split-operator technique for wave packet propagation in quantum systems is expanded here to the case of propagating wave functions describing Schrödinger particles, namely, charge carriers in semiconductor nanostructures within the effective mass approximation, in the presence of Zeeman effect, as well as of Rashba and Dresselhaus spin-orbit interactions. We also demonstrate that simple modifications to the expanded technique allow us to calculate the time evolution of wave packets describing Dirac particles, which are relevant for the study of transport properties in graphene.

PACS: 73.21.Hb, 73.63.Nm, 73.43.Cd

Key words: Wave packet propagation, spin-orbit coupling, graphene, semiconductor heterostructures.

1 Introduction

The time evolution of wave packets is clearly an useful tool in the study of electronic and transport properties of low dimensional systems. Investigating the propagation of wave packets in a given system allows us to obtain information about, e.g., its energy spectrum, [1] its electric and optical conductivity, [2] its local density of states [3] and so on. In fact, wave packet dynamics methods have been successfully used in the study of the Aharonov-Bohm effect in several systems, [4–7] in the theoretical description of scanning gate microscopy experiments, [8] in understanding the break of Onsager symmetry

*Corresponding author. *Email addresses:* andrey@fisica.ufc.br (A. Chaves), gil@fisica.ufc.br (G. A. Farias), francois.peeters@uantwerpen.be (F. M. Peeters), robson.ferreira@lpa.ens.fr (R. Ferreira)

in a semiconductor quantum wire coupled to a metal, [9] and in the interpretation of interference related effects in the experimentally obtained conductance of an asymmetric quantum ring, [10] just to mention a few examples. Lately, the interest in wave packet dynamics methods for Dirac particles has been increasing as well, [11, 12] specially after the first experimental realization of graphene, [13] a single layer of carbon atoms where low energy electrons behave as massless Dirac Fermions, thus exhibiting a series of interesting transport phenomena, such as the zitterbewegung (trembling motion) [14–16] and Klein tunneling [17].

Several computational techniques have been developed for calculating wave packet propagation in quantum structures [18, 19]. In fact, it is clear that, provided one has all the eigenenergies and eigenfunctions of the system, it is always possible to expand the initial wave packet in the eigenstates basis and then calculate its time evolution. However, obtaining the whole spectrum of a system is usually not an easy task, therefore, it is more convenient to look for alternative solutions to the time-dependent Schrödinger (or Dirac) equation. Most of the alternative techniques are based on the expansion of the time-evolution operator, in order to make it computationally easier to be applied in practical situations. Usual examples of this kind of technique are the Chebyshev polynomials expansion [20,21] and the split-operator technique [1,22,23]. The later is particularly convenient, as it splits the time evolution operator into more simple operators, written only in real or imaginary space, allowing one to avoid writing the momentum as a differential operator that has to be computationally implemented in a finite differences scheme.

In the present work, we expand the well known split-operator technique for the investigation of systems where spin-orbit interactions and Zeeman effect play an important role. Indeed, the propagation of Gaussian wave packets in a spin-orbit coupled two-dimensional electron gas (2DEG) has already been discussed in the literature, [24–26] but only with analytical methods, which, on the one hand are exact calculations but, on the other hand, they lack versatility, as they are normally too specific and problem-dependent. In the expanded split-operator technique developed here, the separation of the time-evolution operator in a series of matrices, each one only in real or reciprocal spaces, allows one to calculate the time evolution of the wave packet without using a finite differences scheme. Moreover, we demonstrate that the matrix representation of the Zeeman and spin-orbit parts of the time evolution operator comes from an *exact* expansion of the exponential involved in this operator, so that the only error involved in the technique, which is proportional to the time step Δt, comes from the splitting of the exponential. Therefore, the error in the calculation is easily controlled just by setting a small value for Δt. We then apply the expanded split-operator technique to several cases, demonstrating the validity and versatility of the method in the study of the cyclotronic motion of electrons in a GaAs 2DEG under an applied magnetic field in the presence of Rashba and Zeeman coupling, as well as in the study of the zitterbewegung and Klein tunneling of wave packets in graphene.