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A split-step numerical method for the time-dependent Dirac equation in 3-D axisymmetric geometry

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ABSTRACT

A numerical method is developed to solve the time-dependent Dirac equation in cylindrical coordinates for 3-D axisymmetric systems. The time evolution is treated by a splitting scheme in coordinate space using alternate direction iteration, while the wave function is discretized spatially on a uniform grid. The longitudinal coordinate evolution is performed exactly by the method of characteristics while the radial coordinates evolution uses Poisson's integral solution, which allows to implement the radial symmetry of the wave function. The latter is evaluated on a time staggered mesh by using Hermite polynomial interpolation and by performing the integration analytically. The cylindrical coordinate singularity problem at $r = 0$ is circumvented by this method as the integral is well-defined at the origin. The resulting scheme is reminiscent of non-standard finite differences. In the last step of the splitting, the remaining equation has a solution in terms of a time-ordered exponential, which is approximated to a higher order than the time evolution scheme. We study the time evolution of Gaussian wave packets, and we evaluate the eigenstates of hydrogen-like systems by using a spectral method. We compare the numerical results to analytical solutions to validate the method. In addition, we present three-dimensional simulations of relativistic laser–matter interactions, using the Dirac equation.

1. Introduction

The Dirac equation is among the most important equations in theoretical physics and chemistry as it gives a quantum relativistic description of fermions such as electrons and quarks. When these particles are moving at very high velocity or when they are bound by very strong classical fields, the non-relativistic modeling based on the Schrödinger equation fails and theoretical investigations should be based on the Dirac equation. The extreme conditions where relativistic effects are important can be found in many areas such as relativistic heavy ion collisions, heavy ion spectroscopy, cosmology, astrophysics, and more recently, in laser–matter interactions (for a review, see [1] and references therein) and condensed matter physics [2]. For this reason, the Dirac equation, coupled to an electromagnetic field, has been studied extensively to evaluate many observables such as electron–positron production, molecule spectra, molecular ionization rates, and others. However, solving this equation remains a very challenging task because of its intricate matrix structure, its unbounded spectrum (the Dirac operator has negative energy states which forbid the use of naive minimization numerical methods [3]) and its multiscales (typically for the applications of interests in this paper, the electromagnetic field is macroscopic, with

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a time scale of $t_{E\&M} \sim 0.1$–100 fs $= 0.1$–100×10^{-15} s, while the electron motion, as in the *zitterbewegung* process, has a time scale of $t_{el} \sim 1$ zs $= 10^{-21}$ s, [4]).

Existing approaches to tackle these important problems can usually be classified into three categories. The first one is the analytical method which aims at finding closed-form solutions. Although many important problems were treated in this way [4,5], it only allows the study of idealized systems. The second approach is the semi-classical approximation which can be used to study more complex configurations than the analytical method (see [6] for instance). However, it is only valid for a certain range of wave function parameters, which may not be realized in the physical system under study. The last one is based on full numerical approximations which in principle, can be used to investigate any physical systems. However, even on the numerical side, the solution of the Dirac equation is a challenging problem: it requires a lot of computer resources [7] and certain numerical schemes are plagued by numerical artifacts such as the fermion doubling problem [7–10]. Therefore, special cares have to be taken to resolve these issues when solving the Dirac equation numerically for physically relevant systems.

Among the most successful numerical methods solving the Dirac equation, many are based on a split-step scheme (or split-operator method) where the Dirac Hamiltonian is separated in several operators. This has been used in conjunction with spectral schemes in [11–15] for the Dirac equation, in [16,17] to solve the coupled Maxwell–Dirac system of equations and in [18] for the nonlinear Dirac equation. Very accurate results (with spectral convergence) were obtained with these methods. However, one of the main drawbacks is that the computation time scales like $O(N \log N)$ (where N is the number of spatial points in the discretization) as a Fourier transform has to be computed at every time step. Galerkin methods based on basis function expansion and Fourier mapped methods have been utilized in the study of heavy ion collisions and to compute the pair production rate [19,20]. "Real space" methods were also derived using finite element schemes [9,21] and finite difference schemes (both explicit [22] and implicit [23–25]). More specifically, a leapfrog scheme on a staggered grid was recently considered [26]. However, some of these "real space" methods suffer from the fermion doubling problem [8,27] which induces numerical artifacts and can lead to inaccurate solutions. This occurs because the real-time discretization usually modifies the dispersion relation [8] such that traveling wave packets acquire a wrong group velocity. Consequently, the phase of a traveling wave packet cannot be reproduced accurately by numerical methods suffering from fermion doubling, even when the order of convergence is increased [28].

Recently, a simple numerical method was developed which uses a split-step scheme in "real space" and the method of characteristics to evolve the wave function in time, while the space discretization is performed with finite volume elements [29,30]. This numerical scheme has in fact close connections with the Quantum Lattice Boltzmann technique [31]. In this setting, exact solutions in coordinate space can be used in most steps of the splitting (by choosing carefully the time increment δt and the element size a), resulting in a scheme which is free from the fermion doubling problem[1]) and which can be parallelized very efficiently [30]. This makes for a very powerful and robust numerical technique which allows to study physical systems in Cartesian coordinates, in any number of dimensions. However, for 3-D systems, the computational cost is still very important and thus, only short time events can be treated in that case (such as heavy ion collisions which last for approximately $t_{RHIC} \sim 10^{-23}$–10^{-22} s). For longer events, such as laser–matter interactions (with $t_{pulse} \sim 10^{-18}$–10^{-13} s), only 2-D calculations are possible and therefore, different strategies have to be developed to cope with the high computational requirements. One solution is to reduce the 3-D problem to a 2-D problem by using symmetry arguments. In this work, we adopt this point of view and study systems which are azimuthally symmetric. For this reason, we extend the split-step scheme to solve the Dirac equation in cylindrical coordinates.

The rationale to consider this coordinate system is twofold. First, many physical systems of interests have an azimuthal symmetry and thus, can be treated in cylindrical coordinates. Two examples of this are heavy ion collisions at zero impact parameter, and laser–atom interactions in a counterpropagating laser configuration. Second, it reduces the mathematical description of a 3-D system to an equation in 2-D which of course, reduces the computation time significantly. On the other hand, these coordinates introduce new complications in numerical calculations because the Dirac operator acquires singular terms in the coordinate transformation (terms of the form $1/r$ where r is the radial distance). This complicates the numerical evaluation of this operator on the boundary close to $r = 0$ ($\partial\Omega_{r=0,\theta,z}$, where $\Omega_{r,\theta,z}$ is the domain of the wave function and where $r \in \mathbb{R}^+$, $\theta \in [0, 2\pi]$ and $z \in \mathbb{R}$). This problem has been studied for other equations and many solutions were developed for the Navier–Stokes (and other fluid-like) equations, such as the use of pole conditions [32], shifted mesh [33] and series expansion close to the singularity [34]. A treatment of the singularity for the Schrödinger equation in cylindrical coordinates can be found in [35] where it is shown that the accuracy of the numerical solution can be improved by writing the differential operator in "self-adjoint form". Finally, the Dirac equation with finite difference scheme is treated in [22] where a filter is applied at very time-step to get rid of spurious oscillations close to $r = 0$. In this work, we use another approach which consists of a splitting method analogous to the one presented in [29,30] where alternate dimension iteration is performed. The splitting operators are chosen such that all the singular terms are included in the radial evolution operator. The resulting equations can then be transformed into a set of four 2-D scalar wave equations, expressed in polar coordinates. An integral representation of the solution of these equations can then be found: it is the well-known Poisson formula. The latter can be evaluated by interpolating the wave function spinor components

[1] In 1-D, the numerical dispersion relation is the same as the continuum dispersion relation, so there is no fermion doubling. In 2-D and 3-D, the dispersion relation is reproduced exactly for each coordinate direction. The splitting however modifies slightly this relation for the propagation at an angle.