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High-fidelity numerical solution of the time-dependent Dirac equation

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ABSTRACT

A stable high-order accurate finite difference method for the time-dependent Dirac equation is derived. Grid-convergence studies in 1-D and 3-D corroborate the analysis. The method is applied to time-resolved quantum tunneling where a comparison with the solution to the time-dependent Schrödinger equation in 1-D illustrates the differences between the two equations. In contrast to the conventional tunneling probability decay predicted by the Schrödinger equation, the Dirac equation exhibits Klein tunneling. Solving the time-dependent Dirac equation with a step potential in 3-D reveals that particle spin affects the tunneling process. The observed spin-dependent reflection allows for a new type of spin-selective measurements.

1. Introduction

The Dirac equation [8] is a wave equation from the field of quantum dynamics. Unlike the Schrödinger equation, it is consistent with the theory of special relativity. Relativistic effects are prominent for instance in heavy elements, where the Dirac equation correctly predicts the contraction of inner orbitals and the expansion of outer orbitals. In addition to incorporating relativity for electrons in heavy elements, the Dirac equation describes particle spin, which in contrast needs to be prescribed in the Schrödinger equation. Thus, the Dirac equation fully accounts for the fine structure in hydrogen, whereas a relativistic expansion of the Schrödinger equation only captures part of the effect. The arguably most striking difference between the two models, however, is related to quantum tunneling. The Schrödinger equation predicts that particles can tunnel through classically insurmountable potential barriers, but the tunneling probability decays exponentially inside the classically forbidden region. In [19] Klein presented the surprising result that, according to the Dirac equation, the tunneling probability tends to a non-zero limit as the barrier height goes to infinity—a phenomenon known as Klein tunneling. Yet another important feature of the Dirac equation is that it implies the existence of antiparticles.

In recent years, the Dirac equation has successfully been used to model systems which are not intrinsically relativistic, such as graphene [18]. Here the equation is applied phenomenologically and the speed of light is replaced by the saturation velocity of the electrons in the material, the Fermi velocity.

Mathematically, the Dirac equation is a first order hyperbolic system of four equations with complex coefficients. In contrast, the Schrödinger equation is a second order scalar equation that is neither hyperbolic nor parabolic. Hence, although describing similar physics, the two equations have quite different numerical properties. The Schrödinger equation is stiff—the numerical eigenvalues scale as h^{-2}, where h is the grid-spacing—and requires careful treatment of the numerical

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time-integration. For the Dirac equation, on the other hand, an explicit Runge–Kutta time integrator is generally sufficiently efficient.

Efficient simulation of wave propagation problems generally requires numerical techniques capable of accurately propagating disturbances over long distances. It is well known that high-order finite difference methods (HOFDMs) are ideally suited for problems of this type (see the pioneering paper by Kreiss and Oliger [22]). Not all high-order spatial operators are applicable, however. For example, schemes that are G–K–S stable [11], while being convergent to the true solution as $h \to 0$, may exhibit nonphysical solution growth in time [5], thereby limiting their efficiency for longtime simulations. Thus, it is imperative to use HOFDMs that do not allow nonphysical solution growth in time—a property termed "strict stability" [10]. Deriving a strictly stable, accurate, and conservative HOFDM is a significant challenge that has received considerable past attention. (For examples, see [24,40,38,1,3,13,39,12].)

A robust and well-proven high-order finite difference methodology that ensures the strict stability of time-dependent partial differential equations is the summation-by-parts–simultaneous approximation term (SBP-SAT) method. The SBP-SAT method combines semi-discrete operators that satisfy a summation-by-parts (SBP) formula [21] with physical boundary conditions imposed using the simultaneous approximation term (SAT) method [5]. Examples of the SBP-SAT approach can be found in [33–35,27,29,30,36,26,41,23,7,28,15,14,17].

An added benefit of the SBP-SAT method is that it naturally extends to multi-block geometries while retaining the essential single-block properties: strict stability, accuracy, and conservation [6]. Thus, problems involving complex domains or non-smooth geometries are easily amenable to the approach. References [26,29,16,25] report applications of the SBP-SAT method to problems involving nontrivial geometries.

In this paper we shall apply the SBP-SAT method to the Dirac equation and study time-resolved Klein tunneling numerically. Applications of the SBP-SAT method to first order hyberbolic systems with real coefficients, such as the Euler equations, Maxwell's equations, and the elastic wave equation, have been reported in the literature on several occasions. However, the complex coefficients in the Dirac equation necessitate a slight generalization of the method, in particular when boundary and interface conditions are considered. To the best of our knowledge, this is the first time stable high-order accurate finite difference approximations have been applied to the Dirac equation or similar hyperbolic systems with complex coefficients.

In [4] a split operator fast Fourier transform technique was used to solve the Dirac equation and study Klein tunneling in 1-D. There, smooth potentials were considered. The potential step was modeled by a smoothed step function whose turn-on length was successively decreased to approximate a discontinuous potential. A drawback with this approach is that the rapid turn-on must be resolved, which leads to a large number of grid points in space. In this study, we shall instead use a truly discontinuous potential. As we will demonstrate in a convergence study, the discontinuity must be treated with a multi-block interface to preserve high-order accuracy. With the present SBP-SAT method, no extra spatial resolution is required close to the discontinuity.

To elucidate the difference between the Dirac and Schrödinger equations, we shall compare the solutions to the two models for a tunneling problem in 1-D. By varying the energy of the incoming particle, we can quantify relativistic effects. We shall then proceed to study how particle spin affects time-resolved Klein tunneling in 3-D.

The rest of the paper is organized as follows: The Dirac equation is introduced in Section 2. In Section 3 we introduce the SBP-SAT method and apply it to the Dirac equation in 1-D, including boundary and interface conditions. The extension to 3-D is performed in Section 4. The Schrödinger equation is introduced in Section 5. In Section 6 we verify accuracy and stability by numerical studies in 1-D. We also compare the Dirac and Schrödinger equations for the tunneling problem in 1-D. In Section 7 we verify the accuracy properties of the 3-D scheme against an analytical solution and investigate how particle spin affects Klein tunneling in 3-D. Section 8 summarizes the work.

2. The Dirac equation

The Dirac equation for a spin-$\frac{1}{2}$ particle can be written in the form

$$i\hbar\boldsymbol{\psi}_t = \mathbf{H}\boldsymbol{\psi}, \tag{1}$$

where the wave function $\boldsymbol{\psi}$ is a vector with four components and $\hbar = 1.055 \cdot 10^{-34}$ Js is the reduced Planck constant. In the case of a particle influenced by an electric potential U, the Hamiltonian operator $\mathbf{H}$ is given by

$$\mathbf{H}\boldsymbol{\psi} = \left(c\vec{\boldsymbol{\alpha}} \cdot \hat{\mathbf{p}} + mc^2\boldsymbol{\beta} + qU\right)\boldsymbol{\psi}, \tag{2}$$

where c is the speed of light ($c = 2.998 \cdot 10^8$ m/s) and m and q are the mass and electric charge of the particle. Henceforth, we shall assume that the particle in question is an electron. Thus we will use the electron mass ($m = 9.109 \cdot 10^{-31}$ kg) and the negative elementary charge ($q = -1.602 \cdot 10^{-19}$ C). The momentum operator $\hat{\mathbf{p}}$ is given by

$$\hat{\mathbf{p}} = -i\hbar\nabla. \tag{3}$$

The operators $\boldsymbol{\beta}$ and $\vec{\boldsymbol{\alpha}}$ are defined as

$$\boldsymbol{\beta} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$