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A Finite Element Method Solver for Time-Dependent and Stationary Schrödinger Equations with a Generic Potential

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Abstract. A general finite element solution of the Schrödinger equation for a one-dimensional problem is presented. The solver is applicable to both stationary and time-dependent cases with a general user-selected potential term. Furthermore, it is possible to include external magnetic or electric fields, as well as spin-orbital and spin-magnetic interactions. We use analytically soluble problems to validate the solver. The predicted numerical auto-states are compared with the analytical ones, and selected mean values are used to validate the auto-functions. In order to analyze the performance of the time-dependent Schrödinger equation, a traveling wave package benchmark was reproduced. In addition, a problem involving the scattering of a wave packet over a double potential barrier shows the performance of the solver in cases of transmission and reflection of packages. Other general problems, related to periodic potentials, are treated with the same general solver and a Lagrange multiplier method to introduce periodic boundary conditions. Some simple cases of known periodic potential solutions are reported.

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Key words: One dimensional finite element methods, time dependent Schrödinger equation, periodic boundary conditions, quantum computer simulation.

1 Introduction

This work presents a general solver based on finite element methods (FEM) aimed at solving stationary and time-dependent Schrödinger equations. These equations have analytical solutions in only a few known problems, which are used in books on quantum mechanics to illustrate several points of the theory, i.e., the harmonic oscillator, the

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hydrogen-like system, or in the case of dynamical problems, spreading of a traveling wave packet in space and time. More complex potentials require the use of more sophisticated methods, such as perturbation theory, variational methods or numeric approximations. The equation to be solved has the general form (atomic units are used throughout the text):

$$\left(\frac{1}{2}\Delta+V+F(L,S,B,E)\right)\Psi=i\frac{\partial\Psi}{\partial t}, \tag{1.1}$$

where V represents the external potential and the function F is a general expression which may contain interactions between external magnetic or electrical fields, spin orbit coupling, etc. This general equation can be solved using several numerical schemes. Examples of the finite difference approach can be found in [1, 2]. In such references, an explicit Numerov method is used in order to reach a general solution of both stationary and dynamical problems. This method produces good results for the problems treated but requires a double explicit integration of the system over the domain, and incorporates other limitations specific to the numerical tool. Since the seventies, several approaches to quantum mechanical systems applying FEM to atomic and molecular problems in one, two and three dimensions have been developed [3–12]. Many of these aim to solve hydrogen-like systems with radial symmetry [3], problems involving two-dimensional Schrödinger equations [5], or more sophisticated systems such as the Helium ground state or the Lithium ground state after an integration of the equations in three and six dimensions, after choosing adequate changes in the coordinate system [9, 10]. Other work provides more accurate solutions for systems that are difficult to solve analytically, such as atoms in strong magnetic and electrical fields [6, 8] or time-dependent perturbations, systems which are solved to using others techniques like finite differences and spectral analysis and provides a good reference to try a new numerical technique [26, 27]. More advanced studies extend FEM to self-consistent approaches to quantum systems (DFT and TDDFT), to calculate electronic structures and molecular states [11, 12]. Periodic potentials (common in solid-state physics) are treated using FEM for example in [10, 25], where a general approach to solving systems with periodic boundary conditions is reported, with well-behaved solutions. All of these works show that FEM is a powerful tool for spatially integrating the Schrödinger equation with atomic and molecular potentials in several dimensions. It also shows the high accuracy of the method; which is comparable with other approaches to solving the same equations [12]. One of the most important advantages of FEM over the finite difference method is the possibility of choosing completely general discretization of the space domain without any modification of the system. This allows the use of elements of different size, depending on the requirements of the solution. Using this characteristic, it is possible to choose a fine mesh over that portion of the domain where the solutions contain sharp peaks and a coarser mesh near the external boundaries. This reduces the impact of diffusion errors involved in the numerical schema. FEM have further been used to solve the Schrödinger equation with potentials other than those that are atomic or molecular, such as the three-dimensional harmonic oscillator. Reference [13] shows the important