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

A. Soba*

Computer Applications in Science & Engineering, Barcelona Supercomputing Center, c/Jordi Girona, 31, 08034, Barcelona, Spain.

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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

*Corresponding author. *Email address:* alejandro.soba@bsc.es (A. Soba)

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

relation between the type of elements, space discretization of the domain or the interpolation function used, and the accuracy of the results. It is also necessary to take into account that FEM applied to molecular and electronic structures result in an algebraic system of matrices that are a generalized eigenvalue problem, where the mass matrix is definite positive and an optimized iterative method can be used. However, for generic potentials other than Coulomb potentials, the mass matrix is not definite positive and the method for solving the generalized eigensystem needs to be direct. This is computationally demanding when the space domain is discretized with a fine grid or the number of nodes per element is high, which constitutes a serious limitation to reaching an accurate solution.

In this work we present a general solver based on FEM with particular characteristics for the user. The solver allows the inclusion of general terms in the Schrödinger equation, such as spin orbit coupling or external electromagnetic fields. Secondly, a general term for the potential, which allows the problems ranging from square well to the hydrogen-like system to be studied. Thirdly, it allows the election between different coordinate system and symmetries to solve one-dimensional problems. And finally, the solver allows the resolution of time-dependent problems, such as scattering over potential barriers, etc.

2 The general FEM approach to the Schrödinger equation

A variational or weak FEM approach is used in order of reach a numerical approximation of the time-dependent Schrödinger equation (1.1). This approach converts the differential problem into an equivalent integral (weak) formulation. From this point, in order to find an approximate solution, it is necessary to choose a convenient set of strictly local piecewise polynomials to use in the discrete domain [14]. Applying this approach over each element, the wave function is approximated by a local interpolation function where the unknowns are the local nodal values. In this study we chose fifth/sixth degree polynomials characteristic of Lagrangian elements with five/six nodes as the set of basis functions. Two of these are connectivity nodes and the others are internal. Five/six functions are necessary for each element in order to approximate the solution. In general, a Lagrangian basis function of degree p has unitary value at node p and zero value at all other nodes [14, 15]. The projection of every local system into Eq. (1.1) generates a simple matrix relation for each element. In order to construct this, it is necessary to integrate over each element. We performed all the integrations using four or five point Gauss quadrature, depending on the kind of elements that were used. After this, the local matrices are assembled into global matrices in order to build the generalized eigensystem characteristic of these quantum problems. This will have the form:

$$[K][\Psi] = \lambda [M][\Psi], \tag{2.1}$$

where $K(M)$ is the stiffness (mass) matrix and $\Psi(\lambda)$ is the auto-state (auto-energies) of the problem. In the case of FEM a sparse system is obtained. There are a lot of tools for

solving this kind of problem when the matrix M is positive definite [16] or semi-definite [17]. If the potential term does not have this property, a direct solver taken for example from EisPACK [18] can be used. This solver provides all the eigenvalues and respective eigenvectors of the system for general matrices K and M.

The boundary conditions for one-dimensional symmetric problems are reduced to specifying the value of the solution at infinity. In order to approximate the solution for a discrete space, it is necessary to select a suitable value at this point, depending on the particular problem. In a general description, a Dirichlet essential boundary condition is needed in the extreme domain [4, 5, 6]. A general expression of Eq. (1.1) with spherical (N=2, l can take any value) or Cartesian (N=0, l=0) symmetries and rigid wall boundary conditions [4-6] has the form:

$$i\frac{\partial\Psi}{\partial t}=-\frac{1}{r^N}\left(\frac{\partial}{\partial r}r^N\frac{\partial\Psi}{\partial r}\right)-\frac{\ell(\ell+1)}{2r^2}\Psi+V(r)\Psi, \tag{2.2}$$

$$\Psi(|r|\to\infty,0)=0. \tag{2.3}$$

In the stationary case, the first term is $\epsilon\Psi$ and the weak FEM formulation converts the problem to a generalized eigenproblem of determining the approximate eigenvalues (ϵ, energy) and eigenfunctions (Ψ, wave function). In order to achieve an accurate solution in the discrete domain, an adequate number of elements with a suitable choice of size is necessary. Logarithmic meshes with the fine portion covering the part of the solution containing sharper peaks are a common choice [3–10].

In the time-dependent case, in order to work only with real numbers, the complex system is transformed into two coupled real systems. The final expression has the form:

$$\begin{aligned}-\frac{\partial\Psi^I}{\partial t}&=-\frac{1}{r^N}\left(\frac{\partial}{\partial r}r^N\frac{\partial\Psi^R}{\partial r}\right)-\frac{\ell(\ell+1)}{2r^2}\Psi^R+V(r)\Psi^R+\cdots,\\ \frac{\partial\Psi^R}{\partial t}&=-\frac{1}{r^N}\left(\frac{\partial}{\partial r}r^N\frac{\partial\Psi^I}{\partial r}\right)-\frac{\ell(\ell+1)}{2r^2}\Psi^I+V(r)\Psi^I+\cdots,\end{aligned} \tag{2.4}$$

where $\Psi=\Psi^R+\Psi^I$ and the coupled equations after discretization, result in an asymmetrical non-linear system of matrices:

$$\begin{bmatrix} K(\Psi^R) & -M(\Psi^I)\\ M(\Psi^R) & K(\Psi^I)\end{bmatrix}\begin{bmatrix}\Psi^R\\ \Psi^I\end{bmatrix}=\begin{bmatrix}0\\0\end{bmatrix}, \tag{2.5}$$

where K and M are symmetric. A simple change of sign makes the system symmetrical and the general solver equations can then be used.

$$\begin{bmatrix} K(\Psi^R) & -M(\Psi^I)\\ -M(\Psi^R) & -K(\Psi^I)\end{bmatrix}\begin{bmatrix}\Psi^R\\ \Psi^I\end{bmatrix}=\begin{bmatrix}0\\0\end{bmatrix}. \tag{2.6}$$

The advantage of not working with complex numbers is that we can use the same code as that used to solve stationary problems, by just doubling in the matrices and vector

dimensions. Apart from this, standard solvers of matrices could be used. In the case of a general periodic potential which period L, $V(x)=V(x+L)$, the solutions have the Bloch form, i.e. $\Psi_k(x)=u_k(x)\exp(ikx)$ where is a complex periodic function and k represents the wave vector. Including this expression in the stationary equation (2.1) yields the form:

$$-(\frac{1}{2})\frac{\partial^2 u_k}{\partial x^2}+(V(x)+\frac{k^2}{2})u_k-ik\frac{\partial u_k}{\partial x}=\epsilon_{ki}u_k, \tag{2.7}$$

$$u_0=u_L. \tag{2.8}$$

This Schrödinger-like equation is complex, and again it can be reduced by FEM to a generalized eigenproblem. If a simple reduction to real form is made, taking into account that $u_k(x)=u_k^R(x)+iu_k^I(x)$ as in (2.3) we arrive at two real differential equations that we can put in matrix form as:

$$\begin{bmatrix} K & \Delta \\ -\Delta & M \end{bmatrix}\begin{bmatrix} u_k^R \\ u_k^I \end{bmatrix}=\lambda\begin{bmatrix} M & 0 \\ 0 & M \end{bmatrix}\begin{bmatrix} u_k^R \\ u_k^I \end{bmatrix}, \tag{2.9}$$

where the matrix Δ is antisymmetric and corresponds to the discretized terms which contains the first derivatives of $u_k(x)$. Again this transformation allows the use of a general solver of eigensystems with real matrices, but in this case, they are not symmetric. All that is needed now is to introduce the periodic boundary condition into (2.9) using the Lagrange multiplier method. A periodic boundary condition introduces one nodal equation into the system for each periodic node. For example, in a one-dimensional system, $u_k(0)=u_k(L)$, the solution at the first node of the domain needs to be equal to the solution at the last node of the domain, i.e. $u_{k0}=u_{kN}$. This corresponds to a new equation for the system (2.9), or in fact, two new equations which correspond to two boundary conditions that need to be complimented, one to the real and one to the imaginary part. Then two new rows and columns need to be added to (2.9) for each term to have a periodic system parameterized. Each row/column added is all zeros, except in the places corresponding to the periodic nodes, where the equation $u_{k0}-u_{kN}$ needs to be satisfied. As opposed to methods which simply equate the two solutions in the system and reduce the dimension of the matrices, the Lagrange multiplier method increases the dimensions of the problem, which generates not only the appropriate eigenvalues, but the proper eigenfunctions too.

3 Numerical solutions of the stationary case

Two examples were used to check the accuracy of the method and the goodness of the elements and interpolation functions chosen. The first example corresponds to the Pöschl-Teller potential which represent a model of non-linear vibrational modes of a molecule with two atoms, where θ is the angle between the chemical bounds and D the depth of the potential well. This kind of potential has analytical solutions for the auto-energies and respective wave functions [19, 20]. In this case, a one-dimensional scheme over the Schrödinger equation in Cartesian coordinates was used, with five nodes per Lagrangian

element and fourth-order Gaussian quadrature integration. 200 elements with these characteristics divide a domain of 20 atomic units with rigid wall boundary conditions at the extremes. With this numerical treatment, great accuracy is obtained. The expression for this potential is:

$$V(x)=-\frac{D}{\cosh^2(x)},\quad \tanh(x)=\cos(\theta),\quad \infty\leqslant\theta\leqslant+\infty, \tag{3.1}$$

where the auto-energies take the general analytical expression:

$$\begin{aligned}&\Psi_\nu(x)=C_\nu P_{\lambda-1}^{\lambda-\nu-1}(z),\quad z=\tanh(x),\quad E_\nu=-\frac{1}{2}(\lambda-\nu-1)^2,\\&\nu=0,1,\cdots,[\lambda-1]-1,\quad D=\frac{1}{2}\lambda(\lambda-1).\end{aligned} \tag{3.2}$$

Here P are the Legendre functions of the first kind [21]. Fig. 1 shows the normalized numerical and analytical wave functions and their respective auto-energies for the five bounded states, in the case $\lambda=6$. The last graphic shows the first unbounded state. The solution obtained with the same boundary conditions used for the bounded case shows a good answer in the zone of influence of the potential, and the departure from the predicted solution due to the different boundary condition used.

In order to study the convergence and CPU time required in the solution of our system, we implement a comparison of results obtained with different amounts of elements, taking measures of time consumed and the accuracy of the solution obtained. Table 1 shows several grids in where the system were solved and the comparison between the exact solution and the numeric one in the Pöschl-Teller potential case. The same picture was obtained for the different systems studied.

Table 1: CPU's time consumed and relative error in function of the size of the used system.

	81 N	201 N	401 N	601 N	801 N	1001 N
$(S_{exac}-S_{num})/S_{exac}\times 100$	0.0207	1.2×10^{-5}	8.7×10^{-8}	3.4×10^{-9}	3.6×10^{-10}	9.1×10^{-11}
CPU time (sec)	0.2031	2.2968	17.5468	57.6093	147.7500	237.4375

Of course the better precision in the results is obtained with more elements and more nodes by elements. Systems of great sizes will need better solvers for the generalized eigenproblem involved. In our case in order to reach generality and by the fact that we are trying one dimensional problems which have relative small size, a direct solver can be chosen. This solver provides all the Eigenvalues and respective eigenvector of the system for general matrixes K and M. For a system of 10^6 used to arrive to the better results of the problem, 4 minutes of a Pentium 4 are required approximately (Table 1).

In second place a hydrogen-like system is solved using spherical symmetry producing a one-dimensional radial Schrödinger equation, where $V(x)$ is the Coulomb potential [22]. In this case, six nodes per Lagrangian elements were used in order to discretize the

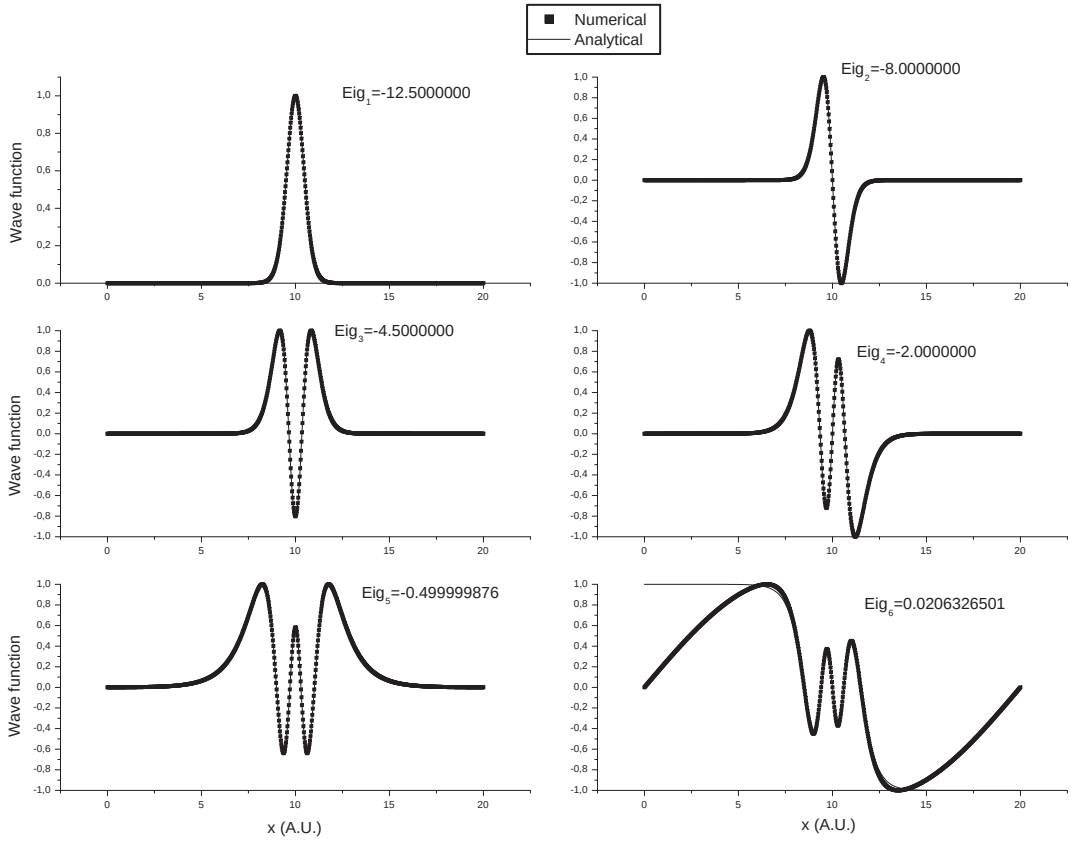

Figure 1: Auto-energies and wave functions of the Pöschl-Teller Potential for $\lambda=6$. The five bound states and the first unbounded state are plotted with the respective auto-energy value obtained numerically.

domain of interest. Fig. 2 shows several principal and orbital quantum number wave functions (normalized) and their respective self-energies are listed. As mentioned above, the accuracy of the solution is highly dependent on the spatial domain over which the equations are defined. It is possible to see that, when the principal quantum number increases, the wave function is more extended in space and the rigid wall condition introduces an error in all the calculations. Extending the domain results in more accurate solutions, as can be seen from Fig. 2c, where for a high principal quantum number the space of integration is greater. Under the same assumption, the error in the auto-energies also increases with the value of the principal quantum number, compared to the theoretical value given by the formula $\epsilon_n = -0.5/n^2$. In each case the first number plotted is almost exact, and deviation increases with each subsequent number. However, this solver allows us to obtain the complete numerical spectra of the hydrogen-like systems just by exploring deferent values of the quantum numbers and taking greater spatial domains. The computational time needed to obtain the spectra in each case is not greater

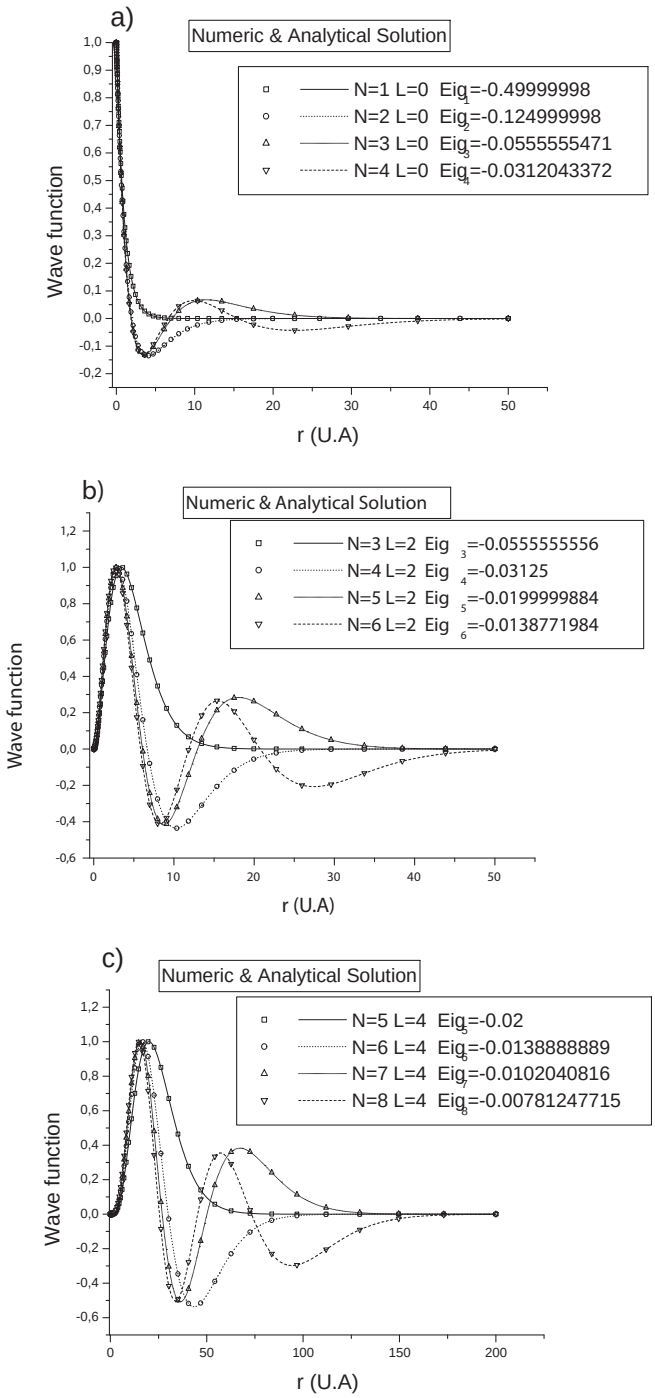

Figure 2: Several auto-functions of the hydrogen-like system for different values of the principal and orbital quantum numbers. The domain of integration needs to be adjusted in each case.

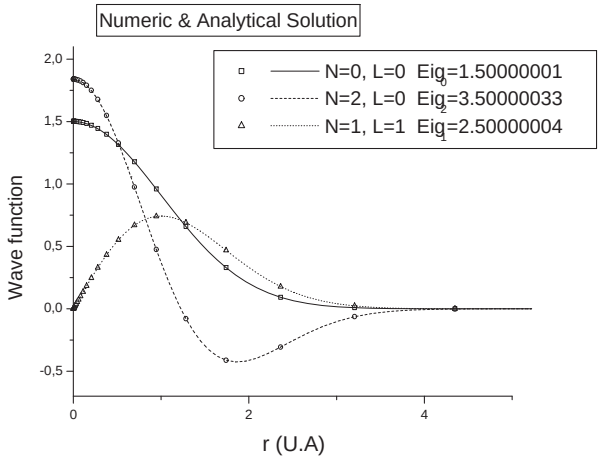

Figure 3: Numerical auto-energies and auto-functions compared with analytic values for the isotropic harmonic oscillator.

than 2 or 3 minutes. In Table 2 the accuracy of the wave function is measured and compared to the analytical value, computing some mean values related to the coordinate r. Again, the two values correspond to a high degree.

Table 2: Numeric and Analytic mean values of $\langle r^2\rangle$, $\langle r\rangle$, $\langle r^{-1}\rangle$, $\langle r^{-2}\rangle$ for several values of N and L. These values show the accuracy of the calculated wave functions.

Num./Anal.	$\langle r^2\rangle$	$\langle r\rangle$	$\langle r^{-1}\rangle$	$\langle r^{-2}\rangle$
N=0, L=0	3.000647/3.0	1.500070/1.5	0.9999566/1.0	1.999512/2.0
N=3, L=2	126.0301/126.0	10.50100/10	0.111105/0.1111	0.01481410/0.0148
N=5, L=4	825.2176/825.0	27.5029/27.50	0.03999788/0.04	0.001777683/0.0018

A general symmetrical isotropic quantum harmonic oscillator is also studied, with a potential given by: $V(r)=-r^2/2$. Both auto-energies and auto-functions depend on the two quantum numbers N and L. In [22] a detailed explanation is given. Fig. 3 shows the first three auto-states with the respective auto-energies obtained numerically. Again, the solution is very accurate compared to similar numeric strategies used for the hydrogen-like system.

4 Numerical solution of the dynamics case

The simplest non-trivial example of a time-dependent quantum wave function is the free Gaussian wave packet [1]. In this case, $V(x)=0$ everywhere and the initial wave is described by:

$$\Psi(x,0)=\exp(ik_0x)\exp\left(-\frac{(x-x_0)^2}{2\sigma^2}\right), \tag{4.1}$$

where the wave package is centered on, $x_0 = 1.0$, $k_0 = 50.0$ represents the velocity group and $\sigma_0 = 0.125$ determines the initial width. Since the package has observable amplitude over the approximate range of $\Delta x = x_0 \pm \sigma(t)$, it is necessary to choose a domain of integration for the Schrödinger equation which is large enough to observe the entire section of interest. In this example a range of 10 atomic units was discretized using Lagrangian elements of five nodes, but the size of the elements was variable: a finer mesh in the central zone, where the oscillation of the solution requires more accuracy, and far away from the centre the elements are larger. Fig. 4 shows different instances of the traveling wave package. The position of the centre of the wave packet coincides with the predicted position according to the analytical expression $(x(t) = tk_0)$.

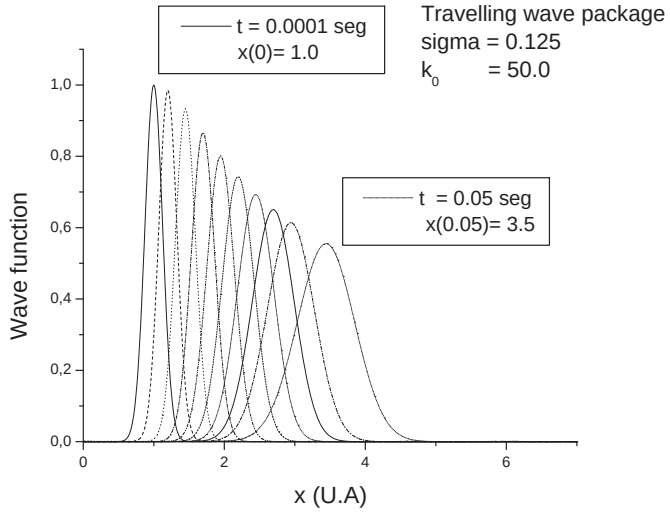

Figure 4: Evolution of a traveling wave packet. Both the center position and dispersion follow those predicted by the analytical formulae.

The next example of a time-dependent Schrödinger equation is a wave packet scattering resonantly from a double rectangular barrier of height 0.25 [1]. We started with an initial Gaussian wave packet centered on $x_0 = 25.0$, and parameters $k_0 = 0.31$, $\sigma_0 = \sqrt{10}$.

The double barrier acts like a filter, transmitting only the energies close to the auto-energies of the potential well formed by the barriers. In the sequences plotted in Fig. 5, it is possible to see an incident wave package, the encounter with the barriers, and subsequent reflected and transmitted packages. The transmitted portion is composed of only those few components in the incident packet with energies within the narrow range of resonance. Long after the main scattering event is over, a small remnant of the initial wave remains trapped between the barriers, steadily losing amplitude. As in the case of a traveling wave packet, the domain considered for the integration has a finer structure close to the barriers and elements of greater size towards both edges, to make the application of a rigid boundary condition possible. Again, this is not a difficult task using FEM and provides good results in both the time-dependent cases shown in this work. The

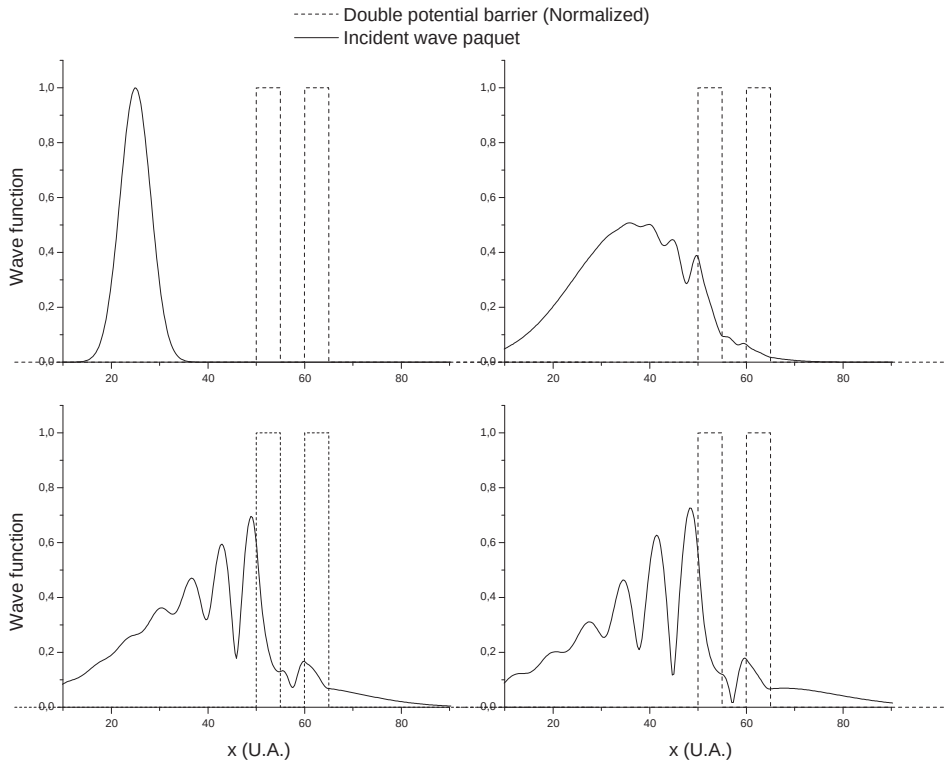

Figure 5: Incident wave packet to a double barrier. In the bottom figures a transmitted and reflected wave packet is showed. It is also possible to see a trapped mode between the barriers.

accuracy of the solution could be compared with several referenced works [28]. Several approaches to related problems can be found in [26, 27] in where a time-splitting spectral scheme are used to solve time dependent Schrödinger equation, using finite difference in space instead FEM.

5 Numerical solution of periodic systems

The simple Kronig-Penney periodic potential is treated with the solver [24]. In this model, the electrons are considered free inside a crystal where the ions have a periodic short-distance interacting potential. The electron is then moved by a periodic one-dimensional lattice with two regions in the unit cell: a zero potential zone of dimension a, and a constant potential zone of dimension b. This potential has an analytical solution and its energy bands are known [24, 25]. Fig. 6 shows a comparison between the numerical and analytical solutions of the bands in function of the wave number k for the following set of parameters: $a = 2a.u.$, $b = 1a.u.$ and $V_0 = 6.5a.u.$ The numerical solutions agree very well with the analytical ones using Lagrangian elements of five nodes and two hundred

elements to discretize the unit cell. Fig. 7 shows several auto-functions for values of the wave number $k=-\pi/(a+b)$ and $k=0.0$ for the first five auto-energies in each case. It is possible to see not only the periodicity of the functions, but also the variation of their form when the value of the potential changes. The values of the auto-energies are listed in each case, showing good agreement with the reported values [24, 25].

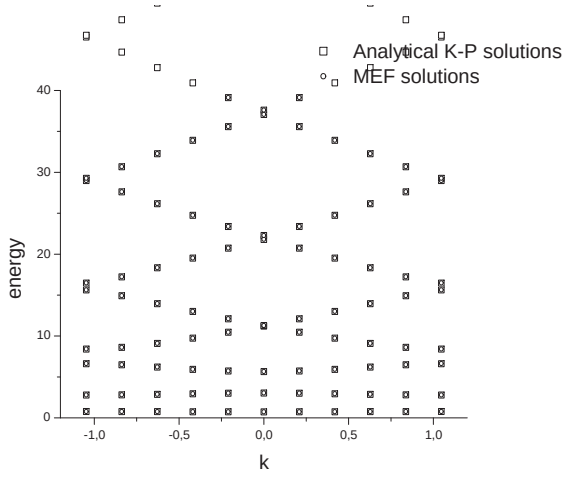

Figure 6: K-P analytical and MEF solutions.

6 Conclusions

We presented a finite element-based solver for generic quantum systems. The solver allows practically all kinds of one-dimensional problems in quantum mechanics related to simple potentials, scattering or interaction between the system and external fields, in different coordinates systems and symmetries to be resolved. The use of Lagrangian elements of five and six nodes shows the best numerical performance in all the cases studied. Throughout the work, the solutions are compared with different known problems with exact analytic solutions and prove to be good approximations. However, it is also possible to use the code with a great variety of potentials with a simple modification. These include perturbed potentials, systems subjected to strong electromagnetic fields, and in general any system without an analytical solution. In the case of periodic and time-dependent problems, converting the system into a real one allows the general real eigen solver to be used, without the need to treat complex numbers. Apart from this, periodic boundary treatments using Lagrange multipliers result in more accurate solutions both for auto-energies and auto-functions, in comparison with more general FEM approaches. The election of proper integration domains and discretization elements allows us to obtain almost all the auto-energies and auto-functions for the potentials studied: the ground states and subsequent exited ones. An extension of the general solver to two- or three-dimensional cases required the use of a fasted solver for eigensystems because

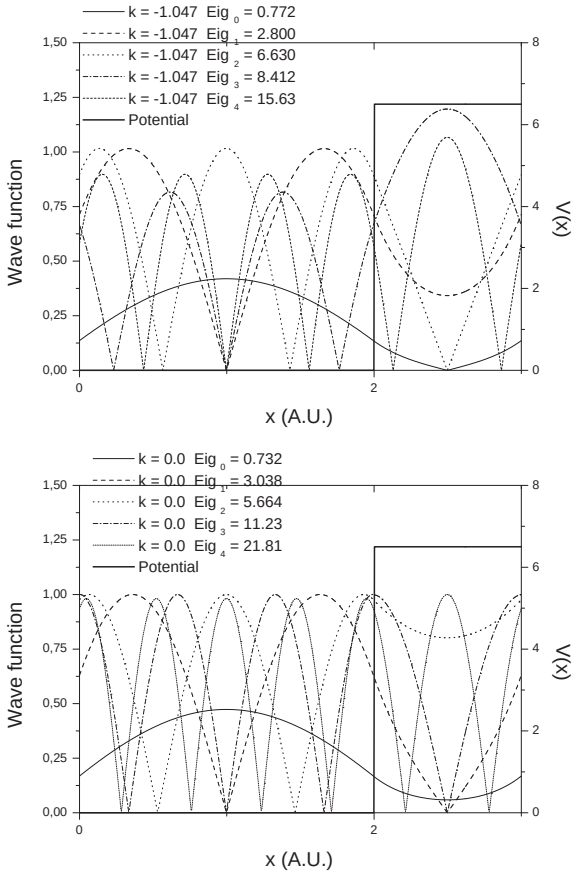

Figure 7: Auto-functions of the Kronig Penney potential for the first five auto-energies for the wave numbers $k=1.047$ and $k=0.0$.

the size of the matrices increases in direct proportion to the number of elements chosen to discretize the space. Part of this final task is still in preparation, and will be published separately.

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