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Dedicated to Professor Dr. Sorin Dan Anghel on His 65th Anniversary

NONUNIFORM NUMERICAL GRID FOR THE NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION

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ABSTRACT. In the present work the numerical grids used during the numerical solution of the Schrödinger equation will be investigated. It will be shown, that by employing a nonuniform optimized numerical grid the number of gridpoints and implicitly the computational effort for the solution of the Schrödinger equation can be significantly reduced. As a test system the harmonic oscillator, and the finite-elements discrete variable representation (FEDVR) numerical will be used, but the obtained results can be extended to other systems and numerical grids too.

Keywords: *ab initio solution of Schrödinger equation, numerical grid optimization, harmonic oscillator*

INTRODUCTION

The processes induced in atomic systems by ultrashort high intensity laser pulses are highly nonlinear [1,2]. The theoretical investigation of these processes (ex. multiphoton ionization, tunneling and over the barrier ionization, high harmonics generation) is a complicated task due to the non-linearity. Since the theoretical models developed for the description of the interaction between traditional light sources (thermal sources, discharge lamps, low intensity lasers, synchrotron radiation) are suitable only for the description of linear processes (i.e. single photon ionization), the development of a new generation of theoretical models became necessary. In the last few decades a large number of theoretical models were developed for the

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theoretical description [1,2] of the above mentioned nonlinear processes, which can be divided into two groups. The first group is formed by the models which are based on the approximate solution of the time-dependent Schrödinger equation. The advantage of these models is that there can be relatively easily computed, and they provide qualitatively good results. However, they have disadvantages too: In most of the cases they do not provide quantitative agreement to the experimental data, and they can not describe all the nonlinear processes simultaneously. The second group is formed by the models, which are based on the *ab initio* numerical solution of the Schrödinger equation. These models provide results with excellent agreement with the experimental data, however, they imply a large computational effort. The Schrödinger equation for systems with a single active particle (electron) can be solved numerically on a simple workstation, however for larger systems with 2 or more active particles high performance computing clusters are required.

The models based on the *ab initio* solution of the Schrödinger equation have two major components: the first is the numerical grid (or numerical basis) on which the wave function is represented, while the second is the method which is used for the time-propagation of the wave function. The optimal implementation of these two components can significantly reduce the computational effort needed for the solution of the Schrödinger equation.

For the time-propagation there is a large set of advanced and highly optimized methods (Crank-Nicolson [3], short-iterative Lánczos [4], Adams-Bashforth-Moulton [5], etc.) available, which can be implemented with adaptive time-steps. In the case of these time propagators there is little room for further optimization. In contrast to this, the currently used numerical grids for the representation of the wave function can be further optimized. Compared to the simplest approach (finite difference representation – i.e. equidistant numerical grid) the more elaborate approaches (b-spline basis [8], finite-element discrete representation – FEDVR [6,7]) perform much better, achieving a significant performance increase of the numerical program. In the atomic physics community the use of FEDVR [6,7] or b-spline [8] discretization is a well spread practice during the numerical solution of the time-dependent Schrödinger equation. In most of these cases the finite elements (FEDVR) or the basis nodes (b-spline) are uniformly distributed. In some cases a denser grid is used in the vicinity of the nucleus, with a monotonously decreasing density as we depart from the center.

Here, in the framework of the FEDVR representation an approach for the further optimization of the numerical grid will be presented. As the result of this optimization, the number of gridpoints (FEDVR basis) which are required for the high precision representation of the ground state wave function of the chosen system (one-dimensional harmonic oscillator) is significantly reduced.

The present work is structured as follows: After this short introduction, in the Theory section, the discretization of the Schrödinger in the FEDVR basis is presented. This is followed by the introduction of the negative imaginary time propagation method, which will be used for the calculation of the ground state of our system. At the end of the section the optimization algorithm is presented. In the next section the numerical convergence test for the homogeneous FEDVR grids and the results of the numerical grid optimization are presented, while in the last section conclusions are drawn. Throughout the paper atomic units are used.

THEORY AND METHODS

In order to test the grid optimization algorithm one of the simplest physical systems, the one dimensional harmonics oscillator was chosen. The Hamiltonian of this system has the following form:

$$\hat{H} = -\frac{\partial^2}{2\partial x^2} + \frac{x^2}{2}, \tag{1}$$

where the mass and the elastic constant of the oscillator is set to 1. The harmonic oscillator was chosen, since the analytical form of it's eigenstates is known, which later on can be used as reference in order to asses the precision of the numerical solution. The stationary Schrödinger equation for our harmonic oscillator has the following form:

$$\hat{H}\psi(x) = E\psi(x), \tag{2}$$

where $\psi(x)$ is the wave function, while E is the energy of the oscillator. The analytical solution of the eigenequation (2) are known. From these solutions the wave function describing the ground state of our oscillator is given:

$$\psi_g(x) = \pi^{-1/4} e^{-x^2/2}. \tag{3}$$

The first step during the numerical solution of Eq. (2) is the discretization of the wave function, i.e. how the continuous wave function is represented by a finite set of real numbers, which can be stored in a computer. Here one of the most advanced discretization approach, the finite element discrete variable representation (FEDVR) is used. In the framework of this approach [6,7,9] the configuration space is divided into finite elements (i.e. into segments with variable length), and inside each segment the wave function is represented in local polynomial basis. The polynomial

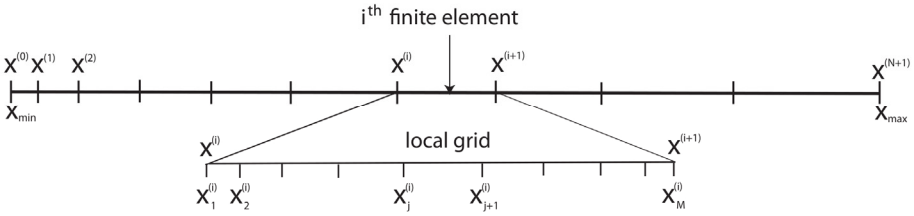

Fig. 1. The illustration of the FEDVR grid

basis functions are built on top of a set of local gridpoints (see Fig. 1), which are chosen to be Gauss integration nodes. For each finite element the Lagrange interpolation polynomials can be written as

$$L_m^{(i)}(x) = \begin{cases} \prod_{j \neq m} \dfrac{x - x_j^{(i)}}{x_m^{(i)} - x_j^{(i)}} & \text{if} \quad x \in \left[x_1^{(i)}, x_M^{(i)}\right] \\ 0 & \text{elsewhere} \end{cases} \tag{4}$$

where $x_j^{(i)}$ are the local gridpoints of the *i*-th finite element, and M is the number of gridpoints (i.e. the number of basis functions) inside the finite element. Using these polynomials the FEDVR basis can be defined as

$$f_m^{(i)}(x) = \begin{cases} \dfrac{L_1^{(i)}(x) + L_M^{(i-1)}(x)}{w_1^{(i)} + w_M^{(i-1)}} & \text{if} \quad m = 1 \\ \dfrac{L_m^{(i)}(x)}{w_m^{(i)}} & \text{if} \quad m = 2, \ldots, M-1 \\ \dfrac{L_M^{(i)}(x) + L_1^{(i+1)}(x)}{w_M^{(i)} + w_1^{(i+1)}} & \text{if} \quad m = M \end{cases}, \tag{5}$$

where $w_m^{(i)}$ are the integration weights corresponding to the $x_m^{(i)}$ quadrature points. With the help of this othonormal basis set the wave function can be expressed as

$$\psi(x) = \sum_{i,j} w_j^{(i)} c_j^{(i)} f_j^{(i)}(x), \tag{6}$$

there the $c_j^{(i)}$ expansion coefficients are simply the value of the wave function in the corresponding gridpoints: $c_j^{(i)} \equiv \psi\left(x_j^{(i)}\right)$. Based on Eq. (6) it can be shown that, as the result of the discretization, the Schrödinger equation (2) is transformed into a matrix eigenequation:

$$H\Psi = E\Psi\Psi \tag{7}$$

where Ψ is the wave function vector (which contains as elements the value of the wave function in the FEDVR gridpoints), and H is the Hamiltonian matrix. This way the solution of the Schrödinger equation is reduced to the solution of a matrix eigenequation, which is standard task in computational sciences. If all the eigenvectors and eigenvalues are sought, then one of the standard linear solvers (lapack [10], SLEPc [11]) can be used, which is a computationally expensive task for a large Hamiltonian matrix. In contrast to this, when only the ground state of a Hamiltonian is searched, an alternative approach, the negative imaginary time propagation (NITP) should be used, which is much less expensive.

In the framework of the NITP approach an arbitrary initial guess of the wave function (ex. a constant function) is propagated in negative imaginary time according to the time dependent Schrödinger equation:

$$-\frac{\partial}{\partial t}\psi(t') = \hat{H}\psi(t'). \tag{8}$$

During this propagation the initial guess will converge towards the ground state wave function of the Hamiltonian. Since the NITP is non-unitary the wave function should be normalized to 1 at each time propagation step.

The precision of the numerically obtained ground state wave function depends on the parameters of the underlying numerical grid on which it is solved. In the case of FEDVR grids, the solution depends on the finite element boundaries, and on the number of basis functions inside the finite elements

$$\psi_g^{num}(x) \equiv \psi_g^{num}\left(x; x_{1,}^{(1)} \ldots, x_M^{(n)}, M\right). \tag{9}$$

Before the optimization of the solution, an optimization parameter should be defined, which can measure the precision of the numerical solution. Based on the exact analytical solution [see Eq. (3)] this measure can be defined as

$$\varepsilon\left(x_1^{(1)}, \ldots, x_M^{(n)}, M\right) \equiv \sum_{i,j} w_j^{(i)} \left|\psi_g\left(x_j^{(i)}\right) - \psi_g^{num}\left(x_j^{(i)}\right)\right|^2, \tag{10}$$

which measures the deviation of the numerical wave function from the analytical one. The goal of the present paper is to find the optimal values for the finite element boundaries, for which ε is minimal.

The optimization algorithm in the present paper is started from a uniform FEDVR grid, where the size of each finite element is the same ($x_m^{(i)} - x_1^{(i)} = \Delta x$). In an optimization loop the position of the finite element boundaries are modified by $\pm \delta x$ one after the other. If as a result of a finite element boundary modification ε decreases, then the modification is accepted, otherwise it is rejected. The optimization loop is repeated until none of the finite element boundary modifications are accepted. Then, the modification step-size is refined ($\delta x \to \delta x / 2$), and the optimization is continued. In the present paper this refinement is applied 5 times after which the optimization is stopped.

RESULTS AND DISCUSSIONS

Since the Hamiltonian of the harmonic oscillator (1) is symmetric with respect to $x = 0,$ the uniform FEDVR grid was chosen to be symmetric too: $x_{min} \equiv x_1^{(1)} = -x_M^{(n)} \equiv x_{max}$, thus the size of the simulation box is $x_{box} = 2x_{max}$, while the size of each finite element is $\Delta x = x_{box} / n.$ For the sake of simplicity, throughout the calculations the number of basis functions inside the finite elements was fixed to $M = 9.$

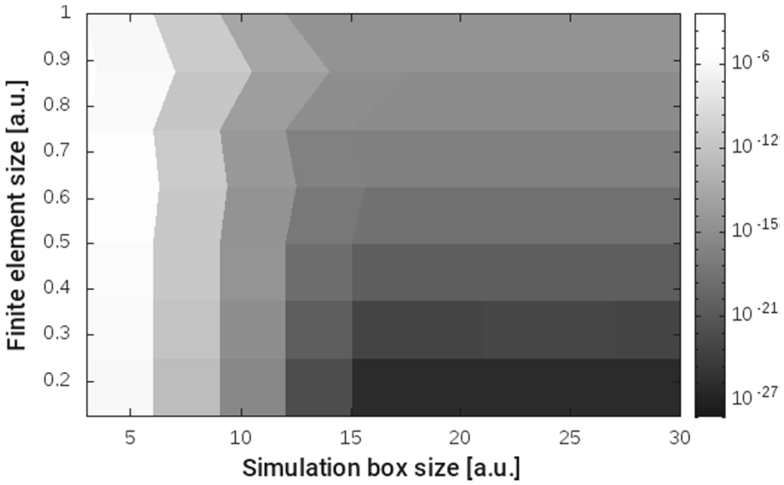

Fig. 2. The precision of the numerical solution (ϵ) as a function of the simulation box size and of the size of the finite element.

Before the application of the optimization algorithm the numerical convergence tests should be performed for the uniform FEDVR grid. The precision of the numerical wave function is shown as the function of the simulation box size (x_{box}) and of the finite element size (Δx) on Fig. 2, where it can be observed the large basin of the parameter space, where the numerical solution is converged. For the better understanding of the convergence properties cuts of the convergence map were prepared. On Fig. 3 the convergence parameter is shown as a function of the finite element size for fixed simulation box size $x_{box} = 30$ a.u. It can be observed that by increasing the density of the numerical grid, the precision of the numerical solution can be increased by orders of magnitude. For the finite element size of 0.125 a.u. the convergence parameter reached the 10^{-26} limit and it's further significant decrease is limited by the double precision floating point representation of real numbers in the computer program. Next, the convergence parameter is shown as a function of the simulation box size for fixed finite element size ($\Delta x = 0.125$). It can be observed the numerical wave function is converging fast as the size of the simulation is increased. For the simulation box sizes larger than 15 a.u. the precision of the numerical wave function can not be increased further, since it is limited by the precision imposed by the numerical grid density.

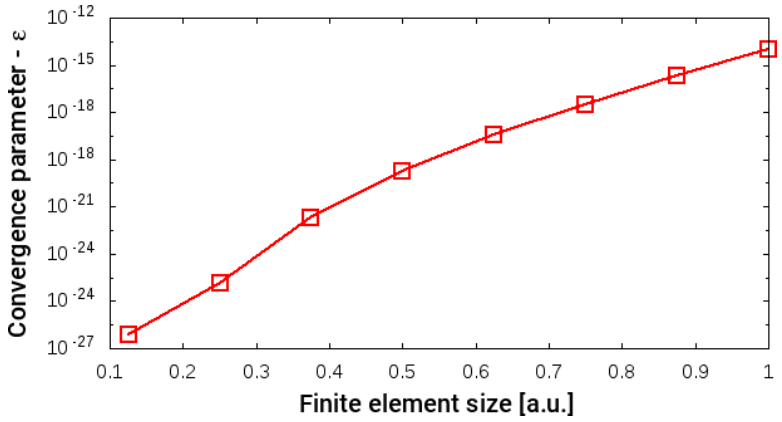

Fig. 3. The precision of the numerical solution as a function of Δx for fixed $x_{box} = 30$ a.u.

Based on the above conclusions the optimization algorithm is applied for a simulation box size fixed at $x_{box} = 16$ a.u. During the optimization the symmetry of

the Hamiltonian is exploited, which reduced significantly the parameter space (the number of free parameters is reduced by half). The initial value of the finite element boundary modification size was set at $\delta x = 0.02$ a.u., which was refined 5 times.

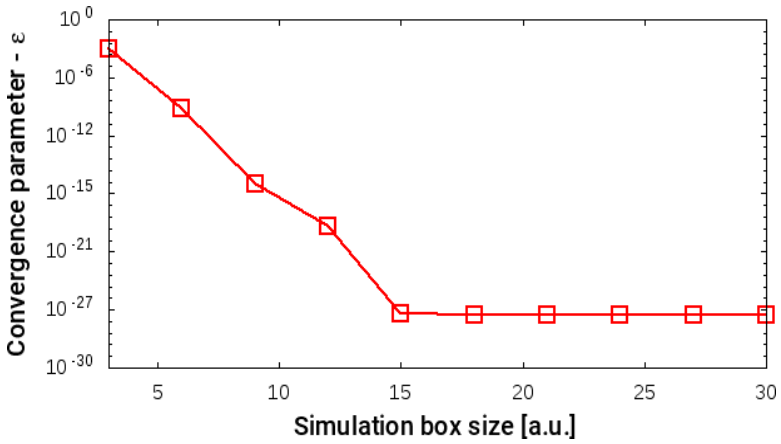

Fig. 4. The precision of the numerical solution as a function of x_{box} for fixed $\Delta x = 0.125$.

The results of the optimization are summarized in Table 1, where for different grid densities (i.e. for different gridpoint numbers N_{gp}) the precision of the of the numerically obtained wave functions are shown for homogeneous (ε_{hom}) and for optimized grids (ε_{opt}). From these results one can observe, that by performing the grid optimization the precision of the obtained numerical wave function can be significantly (by 4 or 5 orders of magnitudes) increased. Or, alternatively, a target wave function precision can be achieved with less gridpoints (i.e. with less computational resources) on an optimized grid. For example the $\varepsilon = 10^{-19}$ target precision can be achieved with 275 points on a homogenous grid, while the same precision can be reached with only 129 points on an optimized grid. At first sight this reduction of gridpoint number by a factor of 2 does not seem significant. However, the computational resource demand of the numerical solution of the Schrödinger equation scales polynomially as a function of the total gridpoint number, which means that in a 3D problem the reduction of the 1D gridpoint number leads to a significant (orders of magnitude) reduction of the computation time.

Table 1. The precision of the numerical solution before and after optimization for different grid densities. The size of the simulation box is fixed at 16 a.u.

Δx	Ngp	ε_{hom}	ε_{opt}	$\varepsilon_{hom} / \varepsilon_{opt}$
2	65	7.24E-011	2.11E-013	343.12
1	129	3.74E-014	3.96E-019	94358.10
0.5	257	2.85E-019	2.35E-023	12131.81
0.25	513	6.44E-024	2.71E-024	2.37

The presented results also show that the optimization does not always leads to significant improvement of the results. When the results are already converged on a homogeneous grid the optimization of the grid does not lead to significant improvements (see the data in the last row of Table 1). In the other extreme case, when the homogeneous grid is sparse, the results of the grid optimization is also less spectacular (see the data in the first row of Table 1).

CONCLUSIONS AND OUTLOOK

In the present work the numerical grids used during the solution of the Schrödinger equation were investigated using as benchmark system the one dimensional harmonic oscillator. For the numerical representation of the wave function, the finite elements discrete variable representation (FEDVR) approach was used, which is one of the most advanced numerical discretization approach currently used by the atomic physics community. In the first step the convergence of the numerical results as a function of grid parameters was investigated in details for homogeneous FEDVR grids. Then, a grid optimization method was implemented, which was used to obtain the ground state of the harmonic oscillator with the same precision as in the case of homogeneous grids, but with much less gridpoints. It was also observed that grid optimization is not efficient if on the original grid the solution is close to the converged one, or the initial grid is to sparse.

It should be mentioned that optimization algorithm used here does not guarantees that the global minimum of $\varepsilon\left(x_1^{(1)},\ldots,x_M^{(n)},M\right)$ is found, it is very likely that it founds only a local minimum. However, even if this happens, the obtained improvement (the reduction of the gridpoint number by a factor of 2) is important, since it can significantly reduce the computational resources needed for the numerical solution of the Schrödinger equation. The optimization method used here can be easily extended to other type of numerical grids (ex. B-spline), and to time-dependent problems.

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