SIMPLE METHOD FOR NUMERICAL SOLVING OF SCHROEDINGER EQUATION FOR HYDROGEN ATOM IN ELECTRIC FIELD

by

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A propagation numerical method for determining energy eigenvalues and eigen wave functions for hydrogen atom in constant and uniform electric field is described in this paper. Solution is presented for 3-D Schroedinger equation in natural parabolic co-ordinate system. Criteria for accepting eigenvalues are introduced, and results are compared with previous papers.

Key words: Schroedinger equation, hydrogen atom, electric field, Euler iterative method

INTRODUCTION

One of the most important partial differential equations in mathematical physics is the Schroedinger equation. It describes the quantum behaviour of some quantum systems [1-3]. This equation has analytical solution for a limited number of potentials [4]. In most cases, the Schroedinger equation can not be solved analytically, and a numerical method must be applied. In principle, there are two groups of numerical methods for solving the Schroedinger equation: propagating method and matrix method. In the first group, the Schroedinger equation is discretised in space. Energy as eigenvalue can be arbitrary chosen. The wave function is then calculated from the Schroedinger equation, by iterative method. Eigenvalue of energy is accepted if the wave function boundary conditions are satisfied [5]. Some of frequently used iterative methods are Euler method, Runge-Kutta method, Finite difference method, *etc*. [6-8]. In the second group of numerical methods, discretised Schroedinger equation is transformed into matrix equation that can be solved numerically [9, 10]. Matrix rank is equal to the number of steps in discretized space.

The propagating method is usually used for calculation of one-dimension equation. The failure of the method could be a long time of computer calculation. In this paper, Euler iterative method has been used to solve the Schroedinger equation for hydrogen in constant and uniform electric field (Stark effect). The Schroedinger equation in parabolic co-ordinates has been used, since it enables separation of co-ordinates in electric field. This decomposes the problem into one independent ordinary differential equation (ODE) over $\phi = (0.\ 2\pi)$, and the system of two ODE over $u = (0, \infty)$, $v = (0, \infty)$, which have common constant parameter. As a solution, eigenvalues of energy and eigenfunctions have been obtained. The objective of this paper is to find an approach for solving three-dimensional Schroedinger equation and to apply it on entangled co-ordinates. This will enable solving of the Schroldinger equation without separation of co-ordinates. Finally, the aim is pointed on determining the accuracy of results according to spatial step segments in discretization and optimising computer time needed for solving the problem.

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METHODOLOGY

The Schroedinger equation for hydrogen atom in uniform and constant electric field, F, in atomic units is [1]

$$\frac{1}{2}\Delta\Psi \quad \frac{1}{r}\Psi \quad Fr\Psi \quad E\Psi \tag{1}$$

where $\Psi \quad \Psi(\vec{r})$ is wave function, Δ – the Laplace's operator, and E – the eigenvalue of energy. In parabolic co-ordinate system r and z can be linked with parabolic co-ordinates u and v [1,3]

$$r \quad \frac{1}{2}(u \quad v) \text{ and } z \quad \frac{1}{2}(u \quad v) \tag{2a}$$

Laplace operator in parabolic coordinates is

$$\Delta \quad \frac{4}{u \quad v}\left[\frac{\partial}{\partial u} \quad u\frac{\partial^2}{\partial u^2} \quad \frac{\partial}{\partial v} \quad v\frac{\partial^2}{\partial v^2}\right] \quad \frac{1}{uv}\frac{\partial^2}{\partial \phi^2} \tag{2b}$$

where spatial domain is $u = (0, \infty)$, $v = (0, \infty)$, $\phi = (0, 2\pi)$

Replacing eqs. (2a) and (2b) into eq. (1), Schroedinger equation in parabolic co-ordinates becomes

$$\frac{4}{u\ v}\frac{\partial}{\partial u}\ u\frac{\partial^2}{\partial u^2}\ \frac{\partial}{\partial v}\ u\frac{\partial^2}{\partial v^2}\ \Psi$$
$$\frac{1}{uv}\frac{\partial^2\Psi}{\partial\phi^2}\ \frac{4}{u\ v}\Psi\ F(u\ v)\Psi\ 2E\Psi \quad (3)$$

Hamilton's operator for hydrogen atom can be represented as the direct product of Hamiltonians of factor spaces over co-ordinates, $\hat{H}\ \hat{H}_u\hat{H}_v\hat{H}_\phi$. Equation (3) can be separated over coordinates introducing wave function as product $\Psi\ \Psi_u\Psi_v\Psi_\phi$, where $\Psi_u\ \Psi(u)$, $\Psi_v\ \Psi(v)$, and $\Psi_\phi\ \Psi(\phi)$. Introducing last expression in eq. (3), one can obtain

$$\frac{1}{\Psi_u}\frac{\partial\Psi_u}{\partial u}\ u\frac{1}{\Psi_u}\frac{\partial^2\Psi_u}{\partial u^2}\ \frac{1}{\Psi_v}\frac{\partial\Psi_v}{\partial v}$$
$$v\frac{1}{\Psi_v}\frac{\partial^2\Psi_u}{\partial v^2}\ \frac{u\ v}{4uv}\frac{1}{\Psi_\phi}\frac{\partial^2\Psi_\phi}{\partial\phi^2}$$
$$1\ \frac{E}{2}u\ \frac{E}{2}v\ \frac{F}{4}(u^2\ v^2)\ 0 \quad (4)$$

Equation (4) is separable over co-ordinates (u, v, ϕ) into three ODE

$$\frac{1}{\Psi_\phi}\frac{\partial^2\Psi_\phi}{\partial\phi^2}\ m^2 \quad (5a)$$

$$\frac{1}{\Psi_u}\frac{\partial\Psi_u}{\partial u}\ u\frac{1}{\Psi_u}\frac{\partial^2\Psi_u}{\partial u^2}\ \frac{m^2}{4u}\ \frac{E}{2}u\ a\ \frac{1}{4}Fu^2\ 0 \quad (5b)$$

$$\frac{1}{\Psi_v}\frac{\partial\Psi_v}{\partial v}\ v\frac{1}{\Psi_v}\frac{\partial^2\Psi_v}{\partial v^2}\ \frac{m^2}{4v}$$
$$1\ a\ \frac{E}{2}v\ \frac{1}{4}Fv^2\ 0 \quad (5c)$$

where m^2 and a are separation constants. Constant a can have values between 0 and 1.

A former set of equations is now

$$\frac{\partial^2\Psi_\phi}{\partial\phi^2}\ m^2\Psi_\phi \quad (6a)$$

$$\frac{\partial\Psi_u}{\partial u}\ u\frac{\partial^2\Psi_u}{\partial u^2}\ \frac{m^2}{4u}\Psi_u$$
$$a\Psi_u\ \frac{E}{2}u\Psi_u\ \frac{1}{4}Fu^2\Psi_u\ 0 \quad (6b)$$

$$\frac{\partial\Psi_v}{\partial v}\ v\frac{\partial^2\Psi_v}{\partial v^2}\ \frac{m^2}{4v}\Psi_v\ (1\ a)\Psi_v$$
$$\frac{E}{2}v\Psi_v\ \frac{1}{4}Fv^2\Psi_v\ 0 \quad (6c)$$

Discretisation of differential equations

The next step is to discretise differential equations given by eqs. (6a) to (6c). Let us introduce new constant in eq. (6a), $C = m^2$

$$\frac{d\Psi_\phi(\phi)}{d\phi}\ C\Psi_\phi(\phi) \quad (7)$$

where $\Psi_\phi(\phi)\ \frac{d\Psi_\phi(\phi)}{d\phi}\ \frac{\Psi_\phi(\phi\ d\phi)\ \Psi_\phi(\phi)}{d\phi}$ is by definition of first derivative. Discrete form of eq. (7) is

$$\Psi_\phi(\phi\ d\phi)\ \Psi_\phi(\phi)\ d\phi C\Psi_\phi(\phi) \quad (8)$$

If $\Psi_\phi(0)$ and its derivation $\Psi'_\phi(0)$ are known at the beginning of domain, and if the value of constant C has some defined value, the value of the first derivative in the next interval segment, $\Psi_\phi(0\ d\phi)$, can be determined. When the first derivative is known, function in the next segment is $\Psi_\phi(0\ d\phi)\ \Psi_\phi(0)\ \Psi_\phi(0)d\phi$. The second derivative in the next segment can then be calculated from eq. (7), $\Psi_\phi(0\ d\phi)\ C\Psi_\phi(0\ d\phi)$. When function Ψ_ϕ, its first and second derivative are known on one segment, this enables calculation of those values in the next segment. Block diagram, which schematically describes the procedure is shown in fig. 1, for general co-ordinate x. Following iterative procedure and moving step by step, function $\Psi_\phi(\phi)$ and its first derivative $\Psi'_\phi(\phi)$ will be known on whole interval ϕ).

Values of $\Psi_\phi(\phi)$ and $\Psi'_\phi(\phi)$ can be determined from boundary conditions and properties of wave function at the beginning of the interval (finite and continuous). Constant C is unknown and can be taken as a parameter. For different values of C, different wave functions are obtained. Wave function must also fulfil boundary conditions at the end of the interval. The procedure is to accept those values of parameter C, for which wave function fulfils boundary conditions at the end of the interval. These wave functions will be eigenfunctions and parameter C which corresponds to eigenfunctions will correspond to quantum number. In the procedure of discretisation it is necessary to choose some finite discrete steps, $d\phi\ \Delta\phi$, which need to be small enough. Boundary conditions impose that, at the beginning of the interval of the co-ordinate ϕ ($\phi = 0$), wave function must be finite and continuous, $\Psi_\phi(\phi) = 1$ and $\Psi'_\phi(\phi)$. Any finite value at the beginning of the interval is satisfactory, since wave function must be normalized. For discrete value of spatial step over ϕ is taken $d\phi = 2\pi/1000$, and constant C is varied from 1 to 40. Figure 1 shows $\Psi_\phi(2\pi)$ *vs.* parameter C, which is the value of wave function at the end of the interval of the co-ordinate ϕ.

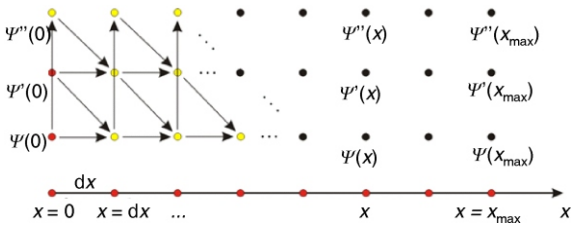

Figure 1. Discretization scheme with algorithm for solving second order ODE for known boundary conditions at the beginning of interval

Wave function Ψ_ϕ must fulfil condition $\Psi_\phi(\phi) = \Psi_\phi(\phi + 2\pi)$, which can be applied on boundary condition, $\Psi_\phi(0) = \Psi_\phi(2\pi)$. From fig. 2 it can be seen that the value of wave function at the end of the interval, $\Psi_\phi(2\pi)$, diverges for $C < 0$. Since it was taken $\Psi_\phi(0) = 1$, we need to find those values of parameters C, for which is $\Psi_\phi(0) = \Psi_\phi(2\pi) = 1$. From fig. 2 it can be seen that this condition is fulfilled for $C = 0, 1, 4, 9, 16, 25, 36, ...$, which are eigenvalues for Ψ_ϕ. Since C is introduced as $C = m^2$, we arrive to quantum number $m = 0, 1, 2, 3, \ldots$ For these values of quantum number, eigenfunctions can be found and are presented in fig. 3.

Eigen problem for co-ordinate ϕ has been solved at this point. Then, eigenvalues and eigenfunctions over co-ordinates u and v have to be found. Equations (6b) and (6c) in discrete form can be written as

$$\Psi_u(u \quad \Delta u) \quad \Psi_u(u) \quad \Delta u \quad \frac{1}{u}\Psi_u(u) \quad \frac{C}{4u^2}\Psi_u(u) \quad \frac{a}{u}\Psi_u(u) \quad \frac{E}{2}\Psi_u(u) \quad \frac{1}{4}Fu\Psi_u(u) \tag{9a}$$

$$\Psi_v(v \quad \Delta v) \quad \Psi_v(v) \quad \mathrm{d}v \quad \frac{1}{v}\Psi_v(v) \quad \frac{C}{4v^2}\Psi_v(v) \quad \frac{1}{v}\frac{a}{}\Psi_v(v) \quad \frac{E}{2}\Psi_v(v) \quad \frac{1}{4}Fv\Psi_v(v) \tag{9b}$$

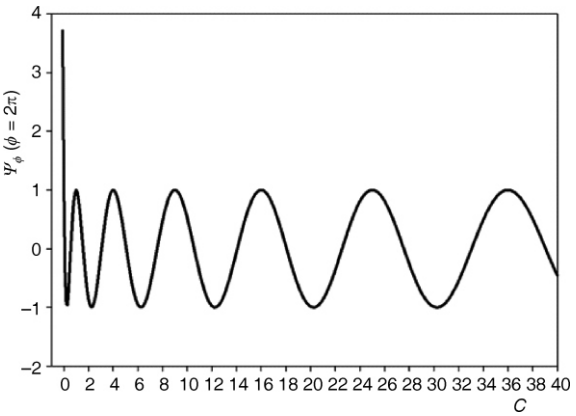

Figure 2. Value of the wave function Ψ_ϕ at the end of the interval, $\Psi_\phi(2\pi)$

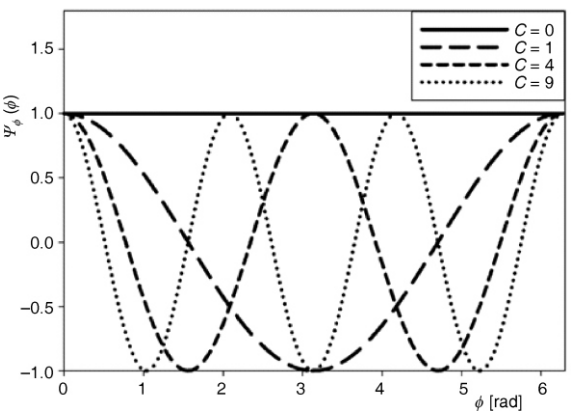

Figure 3. Wave functions Ψ_ϕ for quantum numbers $m = 0, 1, 2, 3$

Previous two equations are not independent and must be solved as a system of two second ODE. The first step is to start without electric field and set $F = 0$. Parameter C is determined from eigen problem over ϕ, and can take values $C = 0, 1, 4, 9, 16, 25, 36, ...$. Let's start from $C = 0$. There are two parameters in eqs. (9a) and (9b) which are unknown, a and E. We need to find those parameters of values a and E, for which, when inserted into (9a) and (9b), boundary conditions over u and v are fulfilled simultaneously. As in the case of co-ordinate ϕ, the following is set: $\Psi_v(0) = \Psi_u(0) = 1$ and $\Psi'_v(0) = \Psi'_u(0) = 0$. Parameter a needs to be varied in range from 0 to 1. Parameter E is not bounded. We need to find those a and E, for which at the end of interval, $u = (0, \infty)$ and $v = (0, \infty)$ wave functions have zero values. Since infinity cannot be reached numerically, we need to set the values for the end of the interval at which behaviour of wave functions is the same as at infinity. We choose $u_{max} = v_{max} = 100$ a. u. (100 Bohr radius) for large enough distance in which wave functions are zero valued. This is fulfilled for ground state and for first three excited states of hydrogen atom, which are examined in this paper. Now, boundary conditions are $\Psi_u(u_{max}) = 0$ and $\Psi_v(v_{max}) = 0$.

To exhibit clearly how eigenvalues of a and E can be found, in figs. 4, 5, and 6 are plotted absolute values $|\Psi_u(u_{max})|$ and $|\Psi_v(v_{max})|$ over a, for $E = -0.49$, $E = -0.5$ and $E = -0.51$, respectively. In iteration procedure, discrete step lengths of u and v are taken to be 10^{-4} a. u.

To present large scale values on plot, logarithmic scale needs to be used. Since negative values cannot be plotted on logarithmic scale, on ordinates of figs. 4 to 6 are presented absolute values of wave functions in logarithmic scale. At points where $|\Psi_u(u_{max})|$ and $|\Psi_v(v_{max})|$ have minimums, wave functions $|\Psi_u(u_{max})|$ and $|\Psi_v(v_{max})|$ actually have zero values and are changing signs. Since from boundary conditions, wave functions on the end of the interval are equal to zero, these minimums of $|\Psi_u(u_{max})|$ and $|\Psi_v(v_{max})|$ correspond to eigenvalue parameters. Since both functions Ψ_u and Ψ_v need to meet boundary conditions for the same values of

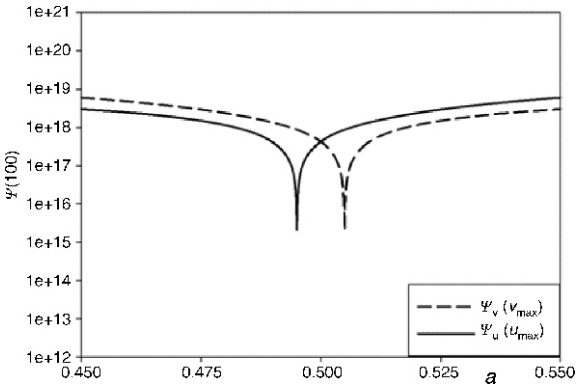

Figure 4. Absolute values of functions $\Psi_u(u_{max})$ and $\Psi_v(v_{max})$, over parameter a, for $u_{max} = v_{max} = 100$ a. u. and $E = -0.49$ a. u.

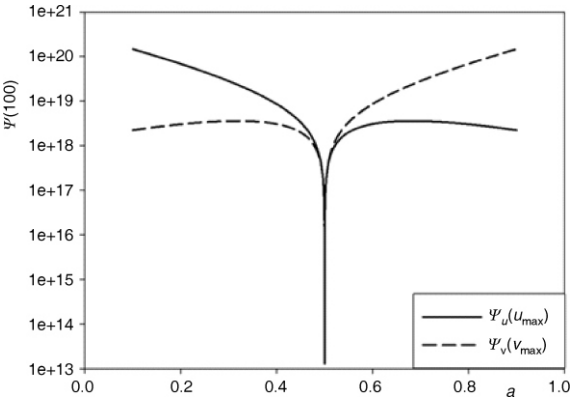

Figure 5. Absolute values of functions $\Psi_u(u_{max})$ and $Y_v(v_{max})$, over parameter a, for $u_{max} = v_{max} = 100$ a. u. and $E = -0.5$ a. u.

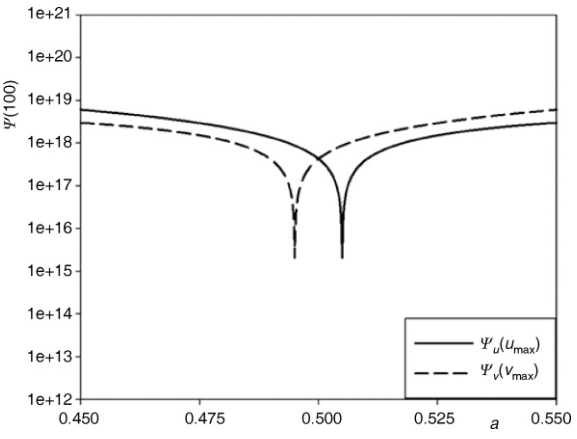

Figure 6. Absolute values of functions $\Psi_u(u_{max})$ and $Y_v(v_{max})$, over parameter a, for $u_{max} = v_{max} = 100$ a. u. and $E = -0.51$ a. u.

a and E, one need to adopt E and a for which both $\Psi_u(u_{max})$ and $\Psi_v(v_{max})$ have zero values. This is the case for eigenvalues in fig. 5. In fig. 4 and 6, both functions Ψ_u and Ψ_v have separate eigenvalues, for different a, and are not eigenfunctions of problem.

In the following text, algorithm for determination of eigenvalues of a and E, for already determined m above, is presented. A general case with external electric field, of strength F, is considered. For atom with no electric field, algorithm is the same, with condition $F = 0$.

Step 1: Set value of electric field, F. Since m is already determined $m = 0, \ 1, \ 2, \ 3$, choose the value for m. For discrete steps of variables u and v, chose small enough dv and du (10^{-4} for 5 digits accuracy, while algorithm runs very fast). For better accuracy, du and dv should be smaller. Maximal value of variables u and v should be set up to $u_{max} = v_{max} = 100$ a. u. for the first three states (for ground state 30 a. u. is large enough).

Step 2: Set the initial value of energy E_{min} and energy step, $dE = -0.01$. This value does not determine energy value accuracy, since it is reduced to a smaller amount in the surrounding of eigen energy.

Step 3: Let us label a with a_u in eq. (9a), and a_v in eq. (9b). Set initial values of a_u, a_v, da_u, and da_v ($da_u = da_v = 0.01$).

Step 4: Set values of wave functions and their derivations at the beginning of intervals, $\Psi_v(0) = \Psi_u(0) = 1$ and $\Psi'_v(0) = \Psi'_u(0) = 0$. Iteratively calculate values of wave functions at the end of intervals $\Psi_u(u_{max})$ and $\Psi_v(v_{max})$, using eqs. (9a) and (9b). Assign obtained values to some variables for storing values, Ψ_{u0} and Ψ_{v0}.

Step 5: For every value of a_v with step da_v, *step 4* is repeated, and obtained values for $\Psi_v(v_{max})$ are compared with Ψ_{v0}. With an increase of a_v, when the condition is fulfilled that function at the end of interval is changing sign, or in other words $\Psi_v(v_{max}) \ \Psi_{v0} < 0$ (changing sign implies that function intercepted ordinate, and went through zero value), then a_v is accepted as an eigenvalue. Go to the next step.

Step 5a: To increase the precision of a_v, return for one step da_v, set $da_v = 0.1\ da_v$, and return to step 5. Step 5a should be run until step size da_v is equal or less than 10^{-7} (for 5 digits accuracy and fast algorithm).

Step 6: Step 5 is now applied on variable u. For each value of a_u with step da_u, step 4 is repeated, and the obtained values of $\Psi_u(u_{max})$ are compared with Ψ_{u0}. With increasing a_u, for some value function at the interval will change sign, $\Psi_u(u_{max}) \ \Psi_{u0} < 0$. Accepted that a_u as eigenvalue.

Step 6a: Apply step 6a on da_u, until the value of 10^{-7} is gained.

Step 7: Find difference $a_r = a_v - a_u$. Change the value of energy E for dE, and repeat the procedure from step 3, to this step. We need to find those E for which $a_r = 0$, or for which values a_u and a_v are the same. If for instance $a_r > 0$ for some E, and with changing E for dE, if parameter a_r becomes $a_r < 0$, then E that causes changing of sing is eigenenergy.

Step 8: To increase the accuracy of E determined in step 7, one needs to return one step dE backward, and set $dE = 0.1\ dE$. Return to step 3, in order to determine eigenvalue E with better precision. Repeat procedure until gain desired precision or $dE \quad 10^{-9}$.

RESULTS

Hydrogen atom without external field ($F = 0$)

In order to obtain eigenvalues and eigenfunctions of hydrogen atom we should start from determined values of constant C, which determines magnetic quantum number. For $C = 0$, parameter a can be in range of 0 to 1. Eigenvalues of parameter a, and energy E can be determined following the above mentioned iteration steps. Energy range is set to be from –0.51 to –0.01 a. u. To visually interpret the results, we introduce new function $\Psi_{u_{max}, v_{max}} \quad |\Psi_u(u_{max}) \ \Psi_v(v_{max})|$. This function has ze-

ros for either $\Psi_u(u_{max}) = 0$ or $\Psi_v(v_{max}) = 0$. From eqs. (6b) and (6c), it could be seen that Ψ_u and Ψ_v should be symmetric in respect to parameter a, in the way that Ψ_u for some a should be the same as Ψ_v for $1-a$. Function $\Psi_{u_{max},v_{max}}$ which depends on a and E, should be symmetric in $(a, E, \Psi_{u_{max},v_{max}})$ plot in respect to plane $a = 0.5$. Zeros of $\Psi_{u_{max},v_{max}}$ are determined with zeros of $\Psi_u(u_{max})$, and $\Psi_v(v_{max})$. Since our condition is that $\Psi_u(u_{max})$ and $\Psi_v(v_{max})$ both have zeros, one should accept those zeros of $\Psi_{u_{max},v_{max}}$ in $(a, E, \Psi_{u_{max},v_{max}})$ plot, where interception of $\Psi_u(u_{max})$ zeros and $\Psi_v(v_{max})$ zeros occurs. In fig. 7, $\Psi_{u_{max},v_{max}}$ is presented for $C = 0$ ($m = 0$). The first eigen energy is –0.5 a. u. for $a = 0.5$. The second eigen energy $E_2 = -0.125$ occurs for a = 0.25 and $a = 0.75$. Other eigenvalues are summarized in tab. 1.

Figure 7 and 8 present plotted values of $\Psi_{u_{max},v_{max}}$ as functions of a and E for the value of parameters $C = 1$ and $C = 4$, respectively. Eigenvalues are summarized in tab. 1.

It is known that in parabolic co-ordinates for hydrogen atom, the following relations between quantum numbers are valid, $n_1 \quad n_2 \quad |m| \quad 1 \quad n$, where n is the main

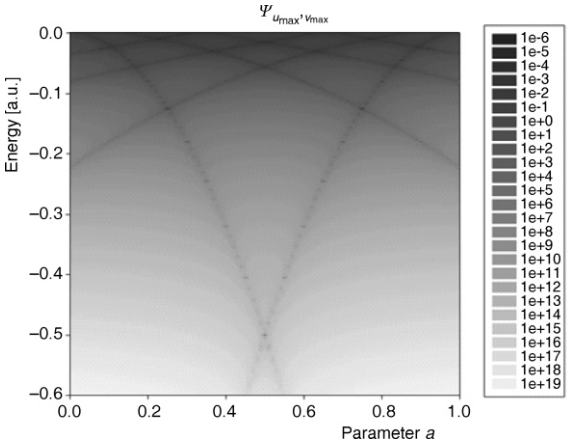

Figure 7. Function $\Psi_{u_{max},v_{max}}$ (a, E), for parameter $C = 0$ ($m = 0$)

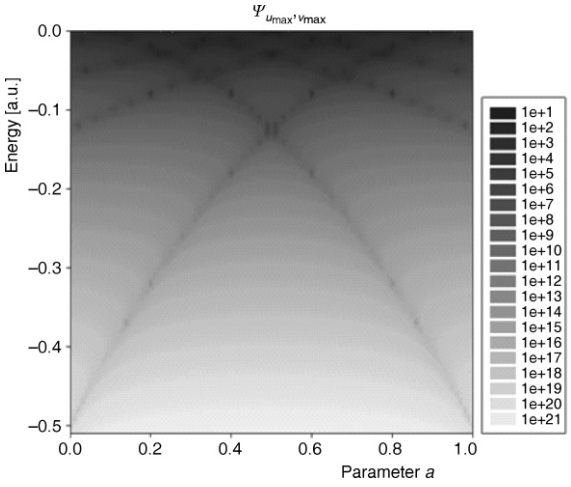

Figure 8. Function $\Psi_{u_{max},v_{max}}$ (a, E), for parameter $C = 0$ ($m = 1$)

Table 1. Summarized eigenvalues of energy and parameter a for $n = 1$, 2, and 3

n	E (a. u.)	a, m
1	–0.5	0.5, $m = 0$
2	–0.125	0.25, $m = 0$
		0.5, $m = 1$
		0.75, $m = 0$
3	–0.0555	0.1667, $m = 0$
		0.3333, $m = 1$
		0.5, $m = 0$, $m = 2$
		0.6667, $m = 1$
		0.8333, $m = 0$
4	–0.03125	0.125, $m = 0$
		0.25, $m = 1$
		0.375, $m = 0$, $m = 2$
		0.5, $m = 1$, $m = 3$
		0.625, $m = 0$, $m = 2$
		0.75, $m = 1$
		0.875, $m = 0$

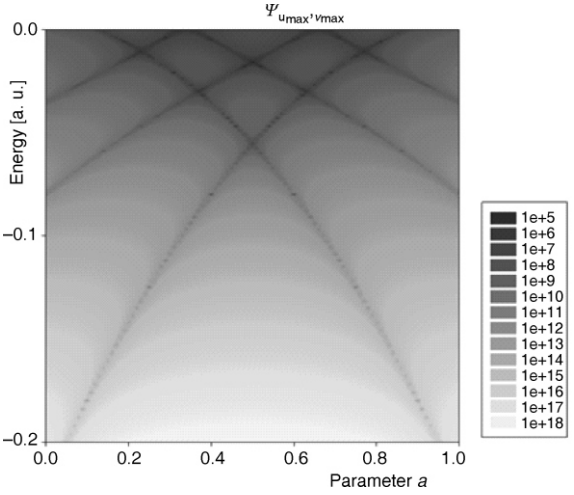

Figure 9. Function $\Psi_{u_{max},v_{max}}$ (a,E), for parameter $C = 4$ ($m = 2$)

quantum number, m is magnetic quantum number and n_1 and n_2 are parabolic quantum numbers [1, 2, 4]. Number of states which is defined by quantum numbers n_1 and n_2 is $n_1 \quad n_2 \quad 1 \quad n \quad |m|$. This is fulfilled from the results obtained in this paper by counting solutions for specified main quantum number (number of states with the same energy) and magnetic quantum number m ($m^2 = C$). For example, for energy $E = -0.125$ a. u. ($n = 2$) and $C = 0$ ($m = 0$), from fig. 5, there are 2 states, which agrees with $n \quad |m| \quad 2$ from theory. Eigenvalues of a for these states are 0.25 and 0.75.

In figs. 10 to 12 are presented eigenfunctions obtained in this paper and compared with analytical solutions.

Hydrogen atom in electric field – Stark effect

Let us introduce external uniform and constant electric field with strength F, defined in atomic units.

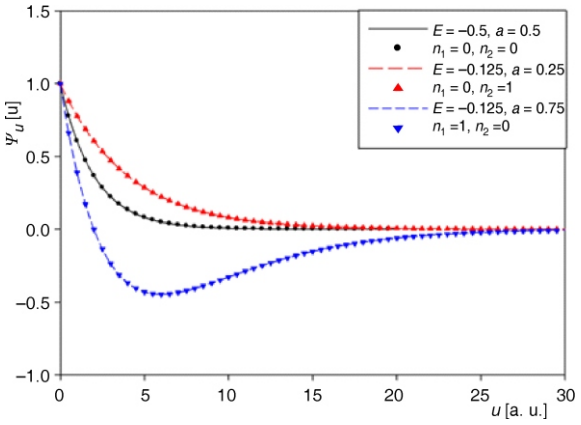

Figure 10. Eigenfunctions presented as continuous lines and comparison with theory [1, 3] given with dots

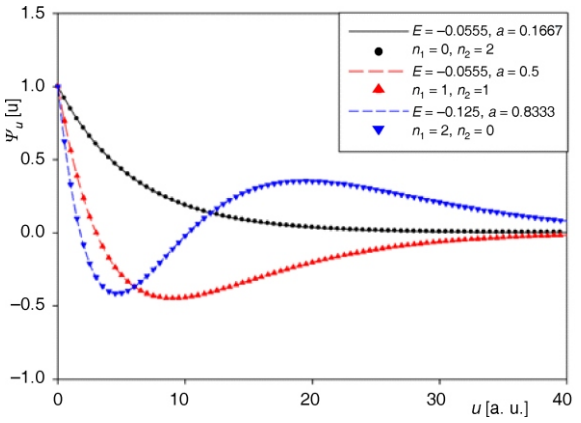

Figure 11. Eigenfunctions presented as continuous lines and comparison with theory [1, 3] given with dots

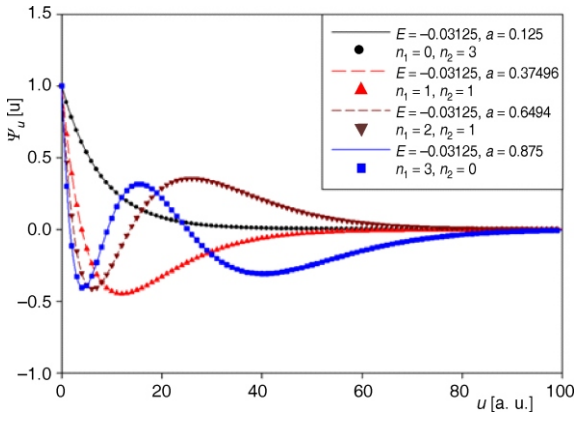

Figure 12. Eigenfunctions presented as continuous lines and comparison with theory [1, 3] given with dots

Electric field, taken to be in *z*-direction cancels degeneracy and shifts eigenenergies. To calculate eigenvalues of energy and parameter *a*, for defined values of electric field *F* we use the procedure described in methodology. Table 2 summarizes the results obtained in this paper, compared with literature values.

In fig. 13, Stark shifting of energies is graphically presented for electric field strength up to 0.005 a. u. for $n = 1, 2$, and 3. The results presented in fig. 13 are the same as in [7], used for comparison.

Table 2. Eigenvalues of Hydrogen energies in Stark effect

n	C	*F*	*E*	*a*
1	0	$5\cdot10^{-3}$	–0.5000563000 [this work]	0.5025003259
			–0.5000553 [9]	
			–0.5000562848 [10]	
2	0	$5\cdot10^{-3}$	–0.14246822 [this work]	0.27510834298 0
			–0.1426204 [9]	
			–0.1426186076 [11]	
			–0.142618607 [12]	
			–0.1426186076 [13]	
			–0.1426188 [14]	
2	0	$5\cdot10^{-3}$	–0.11206044 [this work]	0.77606458807
			–0.1120633 [9]	
			–0.1120619240 [11]	
			–0.112061924 [12]	
			–0.1120619240 [12]	
			–0.12062 [14]	
2	1	$5\cdot10^{-3}$	–0.1271457 [this work]	0.5307046459
			–0.1271464 [9]	
			–0.127146612 [12]	
1	0	$5\cdot10^{-2}$	–0.50611 [this work]	0.5255
			–0.506105425 [12]	
			–0.50610542535 [15]	
			–0.5061054 [16]	
			–0.5061054253626 [17]	
			–0.506105392 [18]	

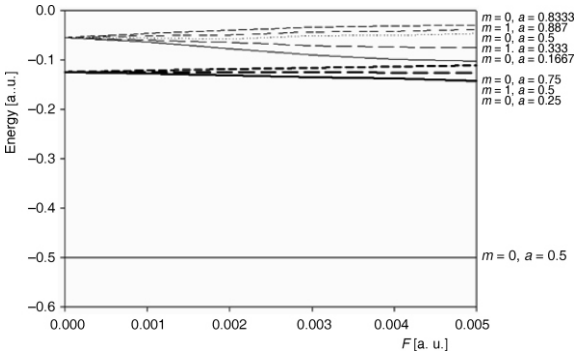

Figure 13. Calculated energies for hydrogen atom as function of electric field strength

CONCLUSION

The aim of this paper is to use the simplest iterative method to find solutions of the Schroedinger equation for hydrogen atom in external constant and uniform electric field. Propagation methods are mostly used to find solutions of one dimensional Schroedinger equations. Here, 3-D partial differential equation is decomposed in parabolic co-ordinates on three ODE, which are not completely independent. Criteria for accepting eigen solutions are introduced in this paper, and the results show that this method can

give accurate results within small computational time, which goes up to several minutes for fixed quantum number m. The accuracy of results can be increased by taking smaller discrete steps during computation. There is no limiting value of electric field strength. Unlike perturbation method, strong field does not have an effect on applicability of the method used in this paper. Another advantage of this method is the possibility to expand its usage to non-separable problems where, instead of separation constant, separation function can be introduced. This function can be determined, as in the case of separation constant, by imposing criteria from boundary conditions. This possibility will be explored in our future work.

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AUUTHORS' CONTRIBUTIONS

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ЈЕДНОСТАВНА МЕТОДА ЗА НУМЕРИЧКО РЕШАВАЊЕ ШРЕДИНГЕРОВЕ ЈЕДНАЧИНЕ ЗА ВОДОНИКОВ АТОМ У ЕЛЕКТРИЧНОМ ПОЉУ

Пропагативна нумеричка метода за одређивање својствене енергије и својствене функције стања водониковог атома у константном и униформном електричном пољу описана је у овом раду. Решење је представљено за тродимензионалну Шредингерову једначину у параболичном координатном систему. Критеријуми за прихватање својствених вредности су уведени и резултати су упоређени са подацима у објављеним радовима.

Кључне речи: Шредингерова једначина, атом водоника, електрично поље, Ојлерова итеративна метода