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ON A METHOD OF SOLVING THE SCHRÖDINGER EQUATION AND ITS APPLICATION IN MODELING THE ELECTRONIC PROPERTIES OF QUANTUM NANOSTRUCTURES

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Abstract. In this paper the numerical techniques for modeling and determining the electronic spectrum and structure of quantum nanostructures is explored. The authors focus on solving the stationary Schrödinger equation using a finite difference scheme. To determine the eigenvalues and eigenfunctions, Danilevsky's method adapted for systems with three-diagonal matrices is developed. The approach is validated through a series of numerical experiments conducted with various input parameter values, demonstrating the robustness and efficiency of the proposed methods. The obtained results can be used for the investigation and optimization of electronic properties of quantum heterostructures.

1. Introduction

The Schrödinger equation is a fundamental equation in quantum mechanics that describes the quantum state of particles with different potentials, including particles confined in a potential well. Solving this differential equation has significant implications in various fields such as atomic physics, molecular physics, solid-state physics, etc.

The stationary Schrödinger equation and the numerical methods for solving it, that is finding eigenvalues and eigenvectors, form an important area of research in quantum mechanics and computational physics. A variety of approaches have been developed to solve these problems, leading to significant progress in both theory and in application. Along with traditional approaches, specialized methods are used to improve computational efficiency and accuracy.

The papers cited below describe various numerical methods and approaches for solving stationary Schrödinger equations and eigenvalue problems, offering a range of techniques that can be applied depending on the specific requirements of the stated problem. Iterative methods such as the Lanczos algorithm and Arnoldi method have gained popularity due to their efficiency in handling large, sparse matrices [1, 9]. They are recommended as a relatively rapid means for determining a small number of larger eigenvalues and modal columns of a large matrix. The eigenstates of the gravitational Schrödinger equation developing a new algorithm to compute these eigenvalues are explored in [3]. This study provides a novel approach to addressing the Schrödinger equation within a gravitational framework, contributing to the understanding of quantum effects in gravitational fields. [13] offers an exact resolution method for the 1D polynomial Schrödinger equation, solving eigenvalue problems with real polynomial potentials. This method stands out for its applicability to a wide range of potential functions. Gusev et al. [6] apply a symbolic-numeric approach to solve boundary-value problems for the Schrödinger equation by using the finite element method. Their work focuses on scattering problems and resonance states, demonstrating the effectiveness of combining symbolic computation with numerical methods. In 2016 Graen and Grubmüller [5] present NuSol, a numerical solver specifically designed for the 3D stationary nuclear Schrödinger equation. Their solver uses advanced techniques, including Krylov subspace methods, to accurately determine eigenvalues and eigenvectors, demonstrating the potential for practical applications in nuclear physics. Sandin, Ögren, and Gulliksson [12] focus on the stationary multicomponent nonlinear Schrödinger equation, particularly under angular

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momentum constraints. Their numerical approach addresses the complexities of nonlinear interactions in quantum systems, contributing to the study of Bose-Einstein condensates and other phenomena. In [7], a numerical study of the Schrödinger–Newton equations is carried out, exploring the implications of coupling Schrödinger equations with gravitational effects. Their research provides insights into the behavior of quantum systems under gravitational influence, particularly in the context of spherically symmetric solutions. In [10], a model reduction approach for computing eigenvalues and eigenfunctions of Schrödinger equations is introduced. The work emphasizes the efficiency of reduced models in solving high-dimensional problems offering a significant computational advantage while maintaining accuracy.

In the present paper, the numerical technique for modeling and determining the electronic spectrum and structure of quantum nanostructures is studied. The authors focus on solving the stationary Schrödinger equation using a finite difference scheme. To determine the eigenvalues and eigenfunctions, we consider Danilevsky's method for systems with three-diagonal matrices. The proposed computational scheme significantly reduces the use of computational resources. The approach is validated theoretically as well as through a series of numerical experiments conducted with various input parameter values, demonstrating the robustness and efficiency of the proposed methods. The obtained results can be used for investigation and optimization of the electronic properties of quantum heterostructures.

2. Problem Formulation and Numerical Model: Reducing a Physical Problem to a Linear Algebra Problem

Let us consider one-dimensional Schrödinger equation that describes the quantum state of a particle confined in a potential well with 1D Coulomb potential inside it. It is represented mathematically as

$$-\frac{\hbar}{2m^*}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x),\quad x\in[-l,l], \tag{2.1}$$

with the boundary conditions

$$\psi(-l)=\psi(l)=0, \tag{2.2}$$

where

$$V(x)=V_0(x)-\frac{1}{\varepsilon[((x-x_0)^2+b)]^{1/2}}$$

with

$$V_0(x)=\begin{cases}0, & -a<x<a,\\ U_0, & x<-a,\ \ x>a.\end{cases}$$

Here $\psi(x)$ is the wave function, $V(x)$ is the potential energy function, E is the energy eigenvalue, $\hbar$ is the reduced Planck's constant, and m^* is the effective mass of the particle, $0<a<l$, ε, b, U_0, x_0 are the given constants.

To solve problem (2.1), (2.2) numerically, the finite difference method is used. First, on the segment $[-l,l]$, we introduce a regular grid

$$\overline{\omega}_h=\big\{x_i=-l+ih,\ \ i=0,1,\dots,N,\ \ hN=l\big\},$$

and approximate problem (2.1), (2.2) by the following homogeneous difference scheme:

$$\Lambda y+\lambda^h y=0,\ \ -l<x_i=ih<l,\ \ y_0=y_N=0,\ \ i=1,2,\dots,N-1, \tag{2.3}$$

where

$$\Lambda y=(y_{\overline{x}})_x-p(x)y,\quad p(x)=\frac{2m^*}{\hbar^2}\,V(x),\quad \lambda=\frac{2m^*}{\hbar^2}\,E.$$

Remark. Note that problem (2.1), (2.2) is a special case of the Sturm–Liouville problem for a second-order ordinary differential equation. The Sturm–Liouville problem, or the problem of finding eigenvalues and corresponding eigenfunctions, is formulated as follows [11]: Determine the values

of the parameter λ (eigenvalues) for which there exist non-trivial solutions (eigenfunctions) to the following homogeneous differential equation (and find these non-trivial eigenfunctions, as well):

$$\begin{gathered}\frac{d}{dx}\left(k(x)\,\frac{du}{dx}\right) - q(x)u + \lambda r(x)u = 0, \;\; 0 < x < 1, \\ u(0) = u(1) = 0.\end{gathered} \tag{2.4}$$

Here, $k(x)$, $q(x)$, $r(x)$ are piecewise smooth functions which satisfy the conditions

$$0 < c_1 \le k(x) \le c_2, \;\; 0 < c_1 \le r(x) \le c_3, \;\; 0 \le q(x) \le c_4,$$

where c_1, c_2, c_3 and c_4 are the constants.

For the approximate solution of problem (2.4), the finite difference method is used and the differential problem is replaced by the difference scheme. For this purpose, on the segment $[0, 1]$, we introduse a regular grid $\overline{\omega}_h = \{x_i = ih,\ i = 0, 1, \ldots, N,\ hN = 1\}$, and approximate problem (2.4) by the following homogeneous difference scheme:

$$\Lambda y + \lambda^h \rho y = 0, \;\; 0 < x_i = ih < 1, \quad y_0 = y_N = 0, \;\; i = 1, 2, \ldots, N-1, \tag{2.5}$$

where it is supposed that $\Lambda y = (a y_{\overline{x}})_x - d(x)y$ represents a homogeneous difference operator with order of approximation $O(h^2)$. Such scheme can be obtained if the scheme coefficients, e.g., are chosen according to the following formulas, in the case of continues initial coefficients

$$a_i = k_{i-1/2} = k(x_i - 0.5h), \quad d_i = q_i, \quad \rho_i = r_i.$$

In the case of piecewise smooth coefficients of (2.4), we can use the expressions

$$\begin{gathered}a_i = 0.5\big(k(x_{i-1/2} - 0) + k(x_{i-1/2} + 0)\big), \\ d_i = 0.5\big(q(x_i + 0) + q(x_i - 0)\big), \quad \rho_i = 0.5\big(r(x_i - 0) + r(x_i + 0)\big).\end{gathered}$$

In [11], one can find other options for selecting the coefficients of the scheme in the case of piecewise smooth coefficients of (2.4).

For the convergence of the difference scheme the following theorem is valid.

Theorem. *If coefficients $k(x)$, $q(x)$ and $r(x)$ of equation* (2.4) *are sufficiently smooth functions, then when $h \to 0$, the solution of the difference scheme* (2.5) *uniformly converges to the solution of the Sturm–Liouville problem* (2.4) *and the following estimation*

$$|\lambda_n^h - \lambda_n| = O(h^2) \;\; \textit{and} \;\; \|y_n - u_n\|_c = O(h^2),$$

is true, where $\{\lambda, u(x)\}$ is the solution of the differential problem (2.4)*, and $\{\lambda_n^h, y_n\}$ is the solution of the difference problem* (2.5)*.*

It is proven [11] that when the coefficients of the initial problem are piecewise smooth, the solution of the difference scheme uniformly converges to the solution of the differential problem with order $O(h)$.

Given the above observation, we can conclude that the solution of the difference scheme (2.3) will uniformly converge to the solution of the differential problem (2.1), (2.2).

The difference problem (2.3) forms a system of linear algebraic equations with a tridiagonal matrix. Accordingly, the following sections will focus on the algorithm for constructing the eigenvalues and eigenvectors for tridiagonal matrices.

3. Eigenvalue Problem. Danilevsky Method for Tridiagonal Matrix

It is almost impossible to specify the best algorithm for finding the eigenvalues of a matrix. Each of these algorithms has its merits and demerits, which should be taken into account when choosing one or another algorithm.

Many numerical methods for solving the eigenvalue problem are based on matrix similarity transformations, which reduce a given matrix to a form whose eigenvalues are relatively easy to find. The matrix similarity transformation does not change the eigenvalues of the matrix, but transforms its eigenvectors according to a certain algorithm. Therefore, if a transformation is selected that allows us

to obtain a matrix whose characteristic polynomial can be easily written, then any standard iterative method can be applied to compute the roots of the resulting characteristic equation.

The efficiency of different methods for writing the characteristic equation can be judged relying on the analysis of several different methods relative to the number of operations required for the implementation of a particular method given in [8]. Namely, among the methods for writing the characteristic equation, starting with fifth-order matrices, Danilevsky's method is the most favorable in terms of the number of operations.

The computational scheme using Danilevsky's method is based on the principal property of similar matrices as they have identical characteristic polynomials. Danilevsky proposed (n-1)-step similarity transformation of the rows of a matrix $A(n \times n)$, starting from the last row, which reduces the given matrix to the so-called canonical Frobenius form [4]

$$\Phi = \begin{bmatrix} p_1 & p_2 & p_3 & \cdots & p_{n-1} & p_n \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

The construction of the characteristic polynomial of the latter matrix is not associated with significant difficulties. Indeed,

$$|\Phi - \lambda E| = \begin{vmatrix} p_1 - \lambda & p_2 & p_3 & \cdots & p_{n-1} & p_n \\ 1 & -\lambda & 0 & \cdots & 0 & 0 \\ 0 & 1 & -\lambda & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 & -\lambda \end{vmatrix}.$$

If we expand this matrix according to the elements of the first row, we finally obtain

$$|\Phi - \lambda E| = (-1)^n \left(\lambda^n - p_1\lambda^{n-1} - p_2\lambda^{n-2} - p_3\lambda^{n-3} - \cdots - p_{n-1}\lambda - p_n\right) = (-1)^n P_n(\lambda),$$

where

$$P_n(\lambda) = \lambda^n - p_1\lambda^{n-1} - p_2\lambda^{n-2} - p_3\lambda^{n-3} - \cdots - p_{n-1}\lambda - p_n.$$

As mentioned above, $P_n(\lambda)$ is also the characteristic polynomial of the matrix A and by finding its roots we can determine the eigenvalues of the initial matrix A.

Thus, our main objective is to construct the Frobenius matrix Φ. The case of tridiagonal matrix is particularly important for us, because the difference scheme (2.3) corresponds to the system of linear equations with such a matrix. Let's rewrite (2.3) in a general form: find the values of the parameter λ for which a non-trivial solution exists for the following system of linear algebraic equations

$$A\vec{x} = \lambda\vec{x}, \;\; A(n \times n),$$

and find this non-trivial solution, as well. Here, A represents a square tridiagonal matrix with elements a_{ij}, $\vec{x}$ is a vector with components $x_1, x_2, \ldots, x_n$. The λ numbers are the eigenvalues of the matrix A, and the corresponding $\vec{x}$ vectors are the eigenvectors. The characteristic equation of the matrix A is $\det(A - \lambda E) = 0$.

4. Computational Scheme

Let's describe the computational scheme of Danilevski's method for the following tridiagonal matrix A

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & \cdots & 0 & 0 & 0 \\ 0 & a_{32} & a_{33} & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & a_{n-2,n-2} & a_{n-2,n-1} & 0 \\ 0 & 0 & 0 & \cdots & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & a_{n,n-1} & a_{nn} \end{bmatrix}.$$

The 1-st step of the transformation $(k = 1)$***:*** Suppose, the leading element $a_{n,n-1} \neq 0$. We will not consider here the case of a zero leading element. Divide last three elements of the $(n-1)$-th column by the leading element $a_{n,n-1}$ and in the resulting matrix subtract the $(n-1)$-th column, multiplied by a_{nn}, from the n-th column. We obtain the following matrix

$$B^{(1)} = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & \cdots & 0 & 0 & 0 \\ 0 & a_{32} & a_{33} & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & a_{n-2,n-2} & \dfrac{1}{a_{n,n-1}}\, a_{n-2,n-1} & -\dfrac{a_{nn}}{a_{n,n-1}}\, a_{n-2,n-1} \\ 0 & 0 & 0 & \cdots & a_{n-1,n-2} & \dfrac{1}{a_{n,n-1}}\, a_{n-1,n-1} & a_{n-1,n} - \dfrac{a_{nn}}{a_{n,n-1}}\, a_{n-1,n-1} \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}.$$

The described process is equivalent to multiplying the matrix A from the right by the transformation matrix M_{n-1}, which is obtained from the identity matrix $(n \times n)$ by replacing the $(n-1)$-th row with the following row

$$\Big\{0, 0, \ldots, 0, \frac{1}{a_{n,n-1}}, -\frac{a_{n,n}}{a_{n,n-1}}\Big\}.$$

It is obtained from the unit matrix by performing the same operations on it. Hence

$$B^{(1)} = AM_{n-1} = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & \cdots & 0 & 0 & 0 \\ 0 & a_{32} & a_{33} & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & a_{n-2,n-2} & b^{(1)}_{n-2,n-1} & b^{(1)}_{n-2,n} \\ 0 & 0 & 0 & \cdots & a_{n-1,n-2} & b^{(1)}_{n-1,n-1} & b^{(1)}_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}.$$

Thus, this transformation changes only the entries from the intersection of $(n-1)$-th and n-th columns and $(n-2)$-th and $(n-1)$-th rows of the matrix A.

In the matrix $B^{(1)}$, we have

$$b^{(1)}_{i,n-1} = (M_{n-1})_{n-1,n-1} \cdot a_{i,n-1}, \quad i = n-2, n-1,$$
$$b^{(1)}_{n-2,n} = (M_{n-1})_{n-1,n} \cdot a_{n-2,n-1}, \quad \text{and} \quad b^{(1)}_{n-1,n} = (M_{n-1})_{n-1,n} \cdot a_{n-1,n-1}.$$

However, the matrix AM_{n-1} obtained through the described process is not similar to the matrix A.

To obtain a matrix that is similar to A and shares the same eigenvalues, we need to multiply AM_{n-1} from the left by the inverse of M_{n-1}, where M^{-1}_{n-1} is obtained from the $(n \times n)$ unit matrix

by replacing the $(n-1)$-th row with the following row

$$\{0, 0, \dots, 0, a_{n,n-1}, a_{n,n}\}.$$

We can easily verify that $M_{n-1}M_{n-1}^{-1} = E$. This multiplication will display only $(n-1)$-th row of the matrix $B^{(1)}$. Then we will have

$$A^{(1)} = M_{n-1}^{-1}AM_{n-1} = \begin{bmatrix} a_{11} & a_{12} & 0 & \cdots & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & \cdots & 0 & 0 & 0 \\ 0 & a_{32} & a_{33} & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & a_{n-2,n-2} & a^{(1)}_{n-2,n-1} & a^{(1)}_{n-2,n} \\ 0 & 0 & 0 & \cdots & a^{(1)}_{n-1,n-2} & a^{(1)}_{n-1,n-1} & a^{(1)}_{n-1,n} \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix},$$

where

$$a^{(1)}_{n-2,j} = b^{(1)}_{n-2,j}, \;\; j = n-1, n,$$

$$a^{(1)}_{n-1,n-2} = a_{n-1,n-2}a_{n,n-1}, \quad a^{(1)}_{n-1,n-1} = b^{(1)}_{n-1,n-1}a_{n,n-1} + a_{n,n}, \quad a^{(1)}_{n-1,n} = b^{(1)}_{n-1,n}a_{n,n-1}.$$

As we can see, we obtained the matrix, where the last row matches the corresponding row of the Frobenius matrix. Thus, the first step of reducing matrix A to the Frobenius form is complete.

Let's continue this process and consider the k-th step.

The k-th step of the transformation $(k = 2, \dots, n-2)$***:*** Suppose, the leading element $a^{(k-1)}_{n-k+1,n-k} \neq 0$. In the resulting matrix of the previous step $A^{(k-1)}$, let's divide the elements of the $(n-k)$-th column by the leading element $a^{(k-1)}_{n-k+1,n-k}$ and in the obtained matrix subtract the $(n-k)$-th column, multiplied by $a^{(k-1)}_{n-k+1,j}$, from the j-th column, $j = n-k+1, \dots, n$.

This trasformation will allert only the entries in the columns from $n-k$ to n, and $(n-k)$-th and $(n-k-1)$-th rows of the the matrix $A^{(k-1)}$. It is equivalent to multiply the matrix $A^{(k-1)}$ from the right by M_{n-k}. The matrix M_{n-k} is obtained from the $(n \times n)$ unit matrix by replacing the $(n-k)$-th row with the following row

$$\left\{0, \dots, 0, \frac{1}{a^{(k-1)}_{n-k+1,n-k}}, -\frac{a^{(k-1)}_{n-k+1,n-k+1}}{a^{(k-1)}_{n-k+1,n-k}}, \dots, -\frac{a^{(k-1)}_{n-k+1,n}}{a^{(k-1)}_{n-k+1,n-k}}\right\}.$$

Thus, in the obtained matrix $B^{(k-1)} = A^{(k-1)}M_{n-k}$,

$$b^{(k-1)}_{n-k-1,j} = a^{(k-1)}_{n-k-1,n-k}(M_{n-k})_{n-k,j}, \;\; j = n-k, \dots, n,$$

$$b^{(k-1)}_{n-k,n-k} = a^{(k-1)}_{n-k,n-k}(M_{n-k})_{n-k,n-k}, \quad b^{(k-1)}_{n-k,j} = a^{(k-1)}_{n-k,j} + a^{(k-1)}_{n-k,n-k}(M_{n-k})_{n-k,j} + a^{(k-1)}_{1j},$$
$$j = n-k+1, \dots, n.$$

The other elements remain the same.

To obtain a matrix that is similar to A and shares the same eigenvalues, we have to multiply $B^{(k-1)}$ from the left by M^{-1}_{n-k}, where it is obtained from the unit matrix $(n \times n)$ by replacing the $(n-k)$-th row with the following row

$$\{0, \dots, 0, a^{(k-1)}_{n-k+1,n-k}, a^{(k-1)}_{n-k+1,n-k+1}, \dots, a^{(k-1)}_{n-k+1,n}\}.$$

We can easily verify that $M_{n-k}M^{-1}_{n-k} = E$. This multiplication will change only the entries in the $(n-k)$-th row of the matrix $B^{(k-1)}$, with indices from $(n-k, n-k-1)$ to $(n-k, n)$. Then we obtain the matrix $A^{(k)}$, where the last k rows matche the corresponding rows of the Frobenius matrix and

$$a^{(k)}_{n-k,j} = a^{(k-1)}_{n-k+1,1}b^{(k-1)}_{n-k,j}, \;\; j = n-k-1, \;\text{ and }\; j = n,$$

$$a^{(k)}_{n-k,j} = a^{(k-1)}_{n-k+1,1}b^{(k-1)}_{n-k,j} + a^{(k-1)}_{n-k+1,j+1}, \;\; j = n-k, \dots, n-1.$$

Let's consider the final step of the transformation.

The $(n-1)$***-th step of the transformation:*** In the final step, the leading element is $a_{21}^{(n-2)} \neq 0$. We multiply the matrix $A^{(n-2)}$ from the right by M_1, and then from the left by M_1^{-1}, where M_1 is obtained from the unit matrix by replacing the first row with the following row

$$\left\{\frac{1}{a_{21}^{(n-2)}}, -\frac{a_{22}^{(n-2)}}{a_{21}^{(n-2)}}, \ldots, -\frac{a_{2,n-1}^{(n-2)}}{a_{21}^{(n-2)}}, -\frac{a_{2n}^{(n-2)}}{a_{21}^{(n-2)}}\right\},$$

and M_1^{-1} is obtained from the unit matrix by replacing the first row with the following row

$$\{a_{21}^{(n-2)}, a_{22}^{(n-2)}, \ldots, a_{2,n-1}^{(n-2)}, a_{2n}^{(n-2)}\},$$

we can easily verify that $M_1 M_1^{-1} = E$. The product $A^{(n-2)}M_1$ will have the form

$$B^{(n-1)} = A^{(n-2)}M_1 = \begin{pmatrix} b_{11}^{(n-2)} & b_{12}^{(n-2)} & \cdots & b_{1,n-1}^{(n-2)} & b_{1,n}^{(n-2)} \\ 1 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix},$$

where

$$b_{11}^{(n-2)} = a_{11}^{(n-2)}(M_1)_{11}, \quad b_{ij}^{(n-2)} = a_{11}^{(n-2)}(M_1)_{1j} + a_{1j}^{(n-2)}, \;\; j = 2, \ldots, n.$$

To ensure the similarity of matrices, we multiply this matrix on the left by M_1^{-1}. As a result, we obtain the matrix

$$A^{(n-1)} = M_1^{-1}M_2^{-1}\cdots M_{n-1}^{-1}AM_{n-1}\cdots M_2M_1$$

which has the canonical form of the Frobenius matrix corresponding to A:

$$A^{(n-1)} = M_1^{-1}B^{(n-1)} = M_1^{-1}M_2^{-1}\cdots M_{n-1}^{-1}AM_{n-1}\cdots M_2M_1$$
$$= \begin{bmatrix} a_{11}^{(n-1)} & a_{12}^{(n-1)} & \cdots & a_{1,n-1}^{(n-1)} & a_{1n}^{(n-1)} \\ 1 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

where

$$a_{1j}^{(n-1)} = a_{21}^{(n-2)}b_{1j}^{(n-2)} + a_{2,j+1}^{(n-2)}, \;\; j = 1, \ldots, n-1, \quad a_{1n}^{(n-1)} = a_{21}^{(n-2)}b_{1n}^{(n-2)}.$$

If we introduce the notation $a_{1j}^{(n-1)} = p_j$, we obtain

$$A \to \Phi = \begin{bmatrix} p_1 & p_2 & \cdots & p_{n-1} & p_n \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix},$$

from which we can derive the characteristic equation of the original matrix

$$\lambda^n - p_1\lambda^{n-1} - p_2\lambda^{n-2} - \cdots - p_{n-1}\lambda - p_n = 0.$$

5. Algorithm for Computing the Eigenvectors

Danilevsky's method facilitates the construction of the eigenvectors of a given matrix A after the eigenvalues have been determined. Suppose, λ is an eigenvalue of the matrix A. It follows that λ is also an eigenvalue of the Frobenius matrix Φ corresponding to A. The eigenvector of the matrix represents the non-zero solution $\vec{y} = (y_1, y_2, y_3, \dots, y_{n-1}, y_n)$ of the system of linear equations $(\Phi - \lambda E)\vec{y} = 0$,

$$\begin{bmatrix} p_1-\lambda & p_2 & p_3 & \cdots & p_{n-1} & p_n \\ 1 & -\lambda & 0 & \cdots & 0 & 0 \\ 0 & 1 & -\lambda & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & -\lambda & 0 \\ 0 & 0 & 0 & \cdots & 1 & -\lambda \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \cdots \\ y_{n-1} \\ y_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix},$$

or

$$\begin{cases} (p_1-\lambda)y_1 + p_2y_2 + p_3y_3 + \cdots + p_{n-1}y_{n-1} + p_ny_n = 0, \\ y_1 - \lambda y_2 = 0, \\ y_2 - \lambda y_3 = 0, \\ \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \\ y_{n-2} - \lambda y_{n-1} = 0, \\ y_{n-1} - \lambda y_n = 0. \end{cases} \tag{5.1}$$

(5.1) represents a homogeneous system of equations with the determinant equal to zero. Let's find its non-trivial solution up to a proportionality coefficient. Suppose that $y_n = 1$. Then

$$y_{n-1} = \lambda,\ y_{n-2} = \lambda^2, \dots,\ y_2 = \lambda^{n-2},\ y_1 = \lambda^{n-1}.$$

Thus, the eigenvector to be searched for is of the form

$$\vec{y} = (\lambda^{n-1}, \lambda^{n-2}, \dots, \lambda^2, \lambda, 1)^T.$$

Let us denote by $\vec{x} = (x_1, x_2, x_3, \dots, x_{n-1}, x_n)^T$ the corresponding eigenvector of the matrix A, then

$$\vec{x} = M_{n-1}M_{n-2}\cdots M_2M_1\vec{y}.$$

$M_1\vec{y}$ will have the following form:

$$M_1\vec{y} = \begin{bmatrix} \frac{1}{a_{21}^{(n-2)}} & -\frac{a_{22}^{(n-2)}}{a_{21}^{(n-2)}} & \cdots & -\frac{a_{2,n-1}^{(n-2)}}{a_{21}^{(n-2)}} & -\frac{a_{2n}^{(n-2)}}{a_{21}^{(n-2)}} \\ 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \cdots \\ y_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{a_{21}^{(n-2)}} \left(\lambda^{n-1} - \sum_{k=2}^{n} a_{2k}^{(n-2)}\lambda^{n-k}\right) \\ \lambda^{n-2} \\ \cdots \\ \lambda^2 \\ \lambda \\ 1 \end{bmatrix} = \begin{bmatrix} x_1 \\ y_2 \\ \cdots \\ y_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix}.$$

Note that the $M_1\vec{y}$ transformation changes only the first coordinate of the vector $\vec{y}$. Similarly, the second coordinate of the vector is transformed by means of the matrix M_2,

$$M_2M_1\vec{y} = \begin{bmatrix} x_1 \\ \frac{1}{a_{32}^{(n-3)}}\left(\lambda^{n-2} - \sum_{k=3}^{n} a_{3k}^{(n-3)}\lambda^{n-k}\right) \\ \lambda^3 \\ \cdots \\ \lambda \\ 1 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ y_3 \\ \cdots \\ y_{n-1} \\ y_n \end{bmatrix}.$$

And so on, using the matrix M_{n-1}, the $(n-1)$-th coordinate of the vector is transformed

$$M_{n-1}M_{n-2}\cdots M_2M_1\vec{y} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 0 & \frac{1}{a_{n,n-1}} & -\frac{a_{nn}}{a_{n,n-1}} \\ 0 & 0 & \cdots & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix}$$

$$= \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_{n-2} \\ \frac{1}{a_{n,n-1}}(\lambda - a_{nn}) \\ 1 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{bmatrix}.$$

Thus, the process of obtaining the eigenvector of the initial matrix A is completed.

Let's write the formulas for computing the components of the eigrenvector separately,

$$\begin{aligned} x_1 &= \frac{1}{a_{21}^{(n-2)}}\left(\lambda^{n-1} - \sum_{k=2}^{n} a_{2k}^{(n-2)}\lambda^{n-k}\right) = \frac{1}{t_{21}}\left(\lambda^{n-1} - \sum_{k=2}^{n} t_{2k}\lambda^{n-k}\right), \\ x_2 &= \frac{1}{a_{32}^{(n-3)}}\left(\lambda^{n-2} - \sum_{k=3}^{n} a_{3k}^{(n-3)}\lambda^{n-k}\right) = \frac{1}{t_{32}}\left(\lambda^{n-2} - \sum_{k=3}^{n} t_{3k}\lambda^{n-k}\right), \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ x_{n-2} &= \frac{1}{a_{n-1,n-2}^{(1)}}\left(\lambda^2 - \sum_{k=n-1}^{n} a_{n-1,k}^{(1)}\lambda^{n-k}\right) = \frac{1}{t_{n-1,n-2}}\left(\lambda^2 - \sum_{k=n-1}^{n} t_{n-1,k}\lambda^{n-k}\right), \\ x_{n-1} &= \frac{1}{a_{n,n-1}}(\lambda - a_{nn}) = \frac{1}{t_{n,n-1}}(\lambda - t_{nn}), \\ x_n &= 1, \end{aligned}$$

where when reducing to the canonical Frobenius form, the matrix T will be filled in step by step, with one row being saved at each step of the process

$$T = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 & 0 \\ t_{21} & t_{22} & \cdots & t_{2,n-2} & t_{2,n-1} & t_{2n} \\ 0 & t_{32} & \cdots & t_{3,n-2} & t_{3,n-1} & t_{3n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & t_{n-1,n-2} & t_{n-1,n-1} & t_{n-1,n} \\ 0 & 0 & \cdots & 0 & t_{n,n-1} & t_{nn} \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 & 0 \\ a_{21}^{(n-2)} & a_{22}^{(n-2)} & \cdots & a_{2,n-2}^{(4)} & a_{2,n-1}^{(4)} & a_{2n}^{(n-2)} \\ 0 & a_{32}^{(n-3)} & \cdots & a_{3,n-2}^{(n-3)} & a_{3,n-1}^{(3)} & a_{3n}^{(n-3)} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & a_{n-1,n-2}^{(1)} & a_{n-1,n-1}^{(1)} & a_{n-1,n}^{(1)} \\ 0 & 0 & \cdots & 0 & a_{n,n-1} & a_{nn} \end{bmatrix}.$$

The above scheme can be applied even in the case of a full matrix A, significantly reducing memory usage when calculating eigenfunctions.

On the other hand, we can use directly the tridiagonal structure of the matrix A. Assume we have already determined all the eigenvalues of the matrix Φ, or what is the same, of the matrix A. Let λ be any eigenvalue of A. Let us denote by $\vec{x} = (x_1, x_2, x_3, \ldots, x_{n-1}, x_n)$ the corresponding eigenvector of the matrix A, which is a non-zero solution of the equation $(A - \lambda E)\vec{y} = 0$,

$$\begin{bmatrix} a_{11}-\lambda & a_{12} & \cdots & 0 & 0 \\ a_{21} & a_{22}-\lambda & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & a_{n-1,n-1}-\lambda & a_{n-1,n} \\ 0 & 0 & \cdots & a_{n,n-1} & a_{nn}-\lambda \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix}. \tag{5.2}$$

(5.2) represents a homogeneous system of equations with the determinant equal to zero. Let's find its non-trivial solution up to a proportionality coefficient. Suppose that $x_n = 1$. We can then solve the resulting system of equations in a backward direction to determine the remaining components of the eigenvector. From the equation $a_{n,n-1}x_{n-1} + (a_{nn} - \lambda)x_n = 0$, we obtain $x_{n-1} = -\frac{a_{nn}-\lambda}{a_{n,n-1}}$, and from the equation $i + 1$, $i = n - 2, \ldots, 1$, we can compute

$$x_i = \frac{-(a_{ii} - \lambda)x_i - a_{i,i+1}x_{i+1}}{a_{i,i-1}}.$$

6. Numerical Results

Let's consider the following physical problem: a hydrogen like atom is in a one-dimensional rectangular box, which models very well any impurity in a semiconductor quantum well [2]. The Schrödinger equation to be solved in atomic units looks as

$$-\frac{1}{2m^*}\frac{d^2\Psi}{dx^2} + v(x)\Psi = E\Psi, \quad x \in [-l, l], \quad l > 0, \tag{6.1}$$

$$\Psi(-l) = \Psi(l) = 0, \tag{6.2}$$

$$v(x) = v_0(x) - \frac{1}{\varepsilon[((x - x_0)^2 + a_B^2)]^{1/2}}, \tag{6.3}$$

where

$$v_0(x) = \begin{cases} 0, & -a < x < a, \\ u_0, & x < -a, \quad x > a, \end{cases} \tag{6.4}$$

$$0 < a < l, \quad a_B = 9.0, \quad \varepsilon = 10.0, \quad m^* = 0.25, \quad u_0 = 0.031,$$

and a, l, x_0 are the given constants. To reduce the physical problem to a linear algebra problem, we rewrite (6.1) in a following form:

$$\frac{d^2\Psi}{dx^2} - 2m^*v(x)\Psi + 2m^*E\Psi = 0, \quad x \in [-l, l].$$

Introducing a grid $\overline{\omega}_h = \{x_i = -l + ih, \ i = 0, 1, \ldots, n, \ hn = l\}$ on the segment $[-l, l]$, we can approximate the problem (6.1)–(6.4) by the following scheme:

$$\Lambda y - \lambda_h y = 0, \quad y_0 = y_n = 0,$$

where y is a vector with the components y_i, $i = 1, \ldots, n-1$, that approximate the function $\Psi(x)$,

$$\Lambda y = (y_{\overline{x}})_x - 2m^* v(x) y, \quad \lambda_h = -2m^* E,$$

and

$$\Lambda = \begin{bmatrix} -2m^*v(x_1) - \frac{2}{h^2} & \frac{1}{h^2} & \cdots & 0 & 0 \\ \frac{1}{h^2} & -2m^*v(x_2) - \frac{2}{h^2} & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & -2m^*v(x_{n-2}) - \frac{2}{h^2} & \frac{1}{h^2} \\ 0 & 0 & \cdots & \frac{1}{h^2} & -2m^*v(x_{n-1}) - \frac{2}{h^2} \end{bmatrix}.$$

The values of E then are calculated from the expression $E = -\frac{\lambda_h}{2m^*}$.

Below, in Tables 1-3, we present the numerical results, that is, the values of two smallest eigenvalues E_1, E_2, and the corresponding normalized eigenfunctions ψ_1 and ψ_2 are given graphically in Figures 1–6) for different values of input parameters a, l and x_0.

TABLE 1

#	a	l	x_0	E_1	E_2
1.1	9.4	29.4	0	0.00650829	0.0406823
1.2	18.9	38.9	0	−0.00177341	0.0187639
1.3	28.3	48.3	0	−0.00403597	0.00916731

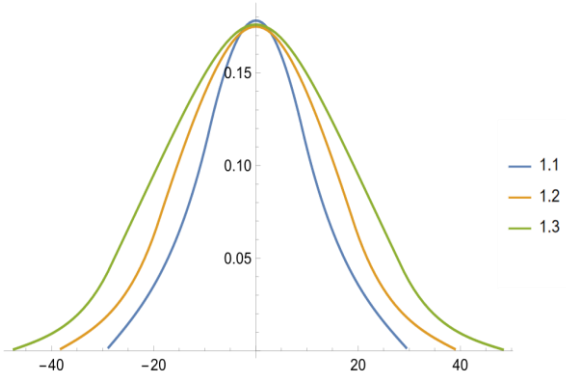


FIGURE 1. ψ_1 for 1.1, 1.2 and 1.3 variants

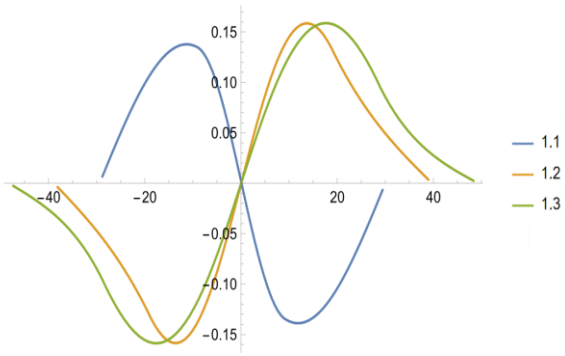


FIGURE 2. ψ_2 for 1.1, 1.2 and 1.3 variants

TABLE 2

#	a	l	x_0	E_1	E_2
2.1	9.4	29.4	−9.4	0.00787984	0.0404619
2.2	18.9	38.9	−9.4	−0.00103017	0.0185145
2.3	28.3	48.3	−9.4	−0.00367912	0.00894366

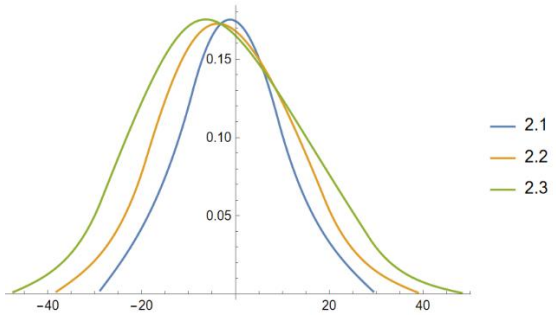


FIGURE 3. ψ_1 for 2.1, 2.2 and 2.3 variants

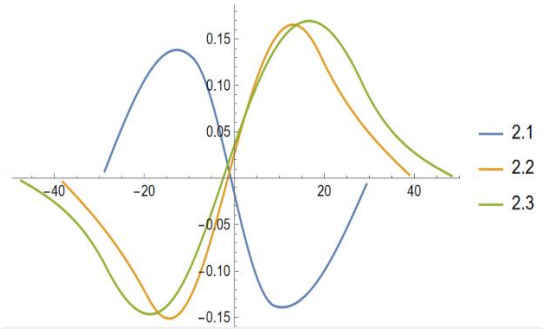


FIGURE 4. ψ_2 for 2.1, 2.2 and 2.3 variants

TABLE 3

#	a	l	x_0	E_1	E_2
3.1	9.4	29.4	-18.9	0.010341	0.0411651
3.2	18.9	38.9	-18.9	0.000896248	0.0188497
3.3	28.3	48.3	-18.9	-0.00252561	0.00879211

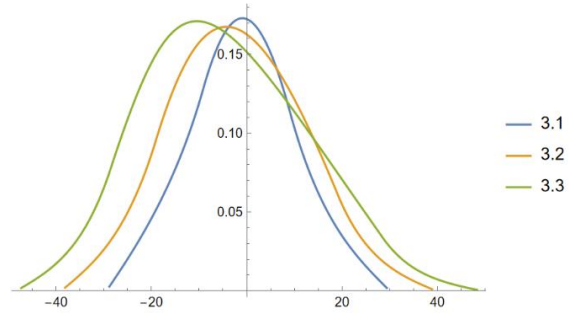


FIGURE 5. ψ_1 for 3.1, 3.2 and 3.3 variants

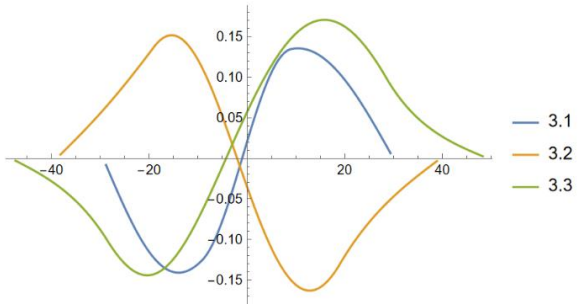
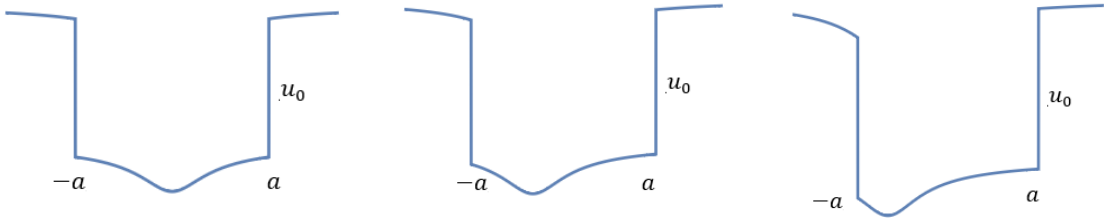


FIGURE 6. ψ_2 for 3.1, 3.2 and 3.3 variants

Figure 7 shows the potential energy function $v(x)$ for the different values of x_0.



var. 1.3, $x_0 = 0$ var. 2.3, $x_0 = -9.4$ var. 3.3, $x_0 = -18.9$

FIGURE 7. $v(x)$ FOR DIFFERENT VALUES OF x_0 (SEE TABLES 1–3).

Figures 8, 9 show the graphs of the eigenfunction corresponding to the two smallest eigenvalues for different values of n (or equivalently, the grid step size h), using the input data from the variant 1.1 (see Table 1).

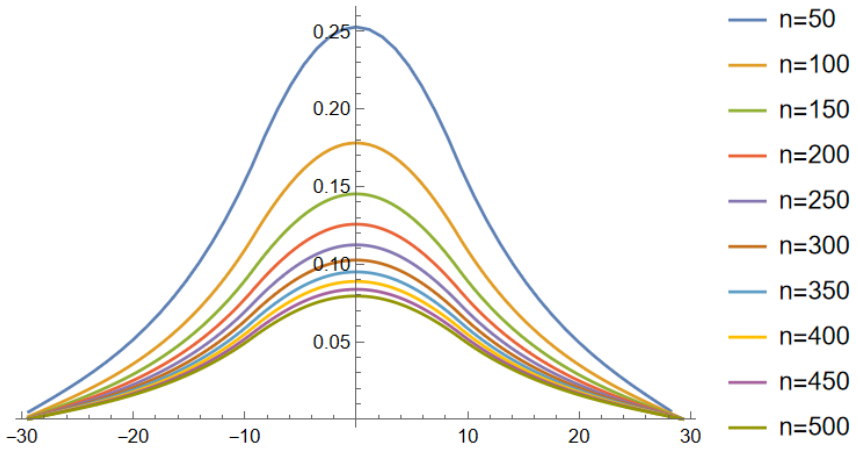


FIGURE 8. BEHAVIOR OF ψ_1 FOR DIFFERENT VALUES OF n.

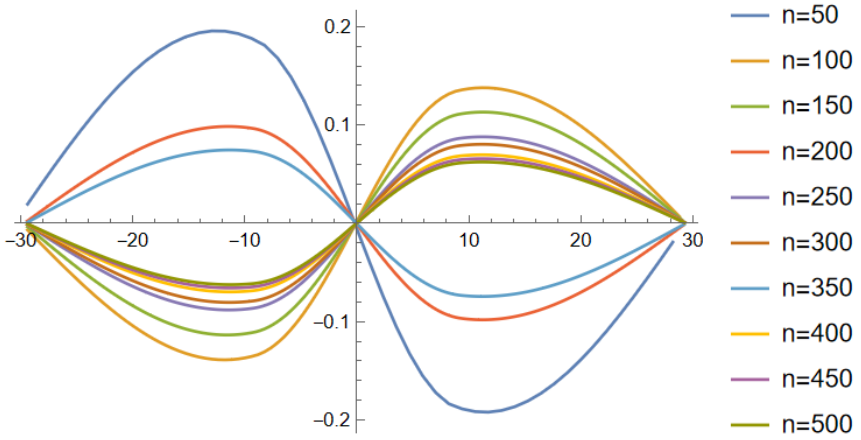


FIGURE 9. BEHAVIOR OF ψ_2 FOR DIFFERENT VALUES OF n.

7. CONCLUSION

This article presents a method for numerical investigating the quantum state of a particle confined in a potential well with 1D Coulomb center, described by the one-dimensional stationary Schrödinger equation. By employing the finite difference method, the spatial domain is discretized, resulting in a linear algebraic system with a tridiagonal matrix. The Danilevsky method was effectively applied to this matrix, enabling the determination of eigenvalues and eigenfunctions with enhanced computational efficiency. The proposed algorithm for eigenfunction computation, characterized by its adaptability to full matrices, significantly reduces memory overhead.

The obtained numerical results confirm the robustness and stability of the proposed method, demonstrating convergence properties that can be applied to the study and optimization of the electronic properties of quantum heterostructures.

Future research will be aimed at generalizing this approach, including investigation of other methods to cover more complex quantum systems, thereby expanding the mathematical and physical insights into quantum mechanical behavior and material characteristics.

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References

1. W. E. Arnoldi, The principle of minimized iteration in the solution of the matrix eigenvalue problem. *Quart. Appl. Math.* **9** (1951), 17–29.
2. K. Barnham, D. Vvedensky, Eds., *Low-Dimensional Semiconductor Structures: Fundamentals and Device Applications*. Cambridge University Press, 1st edition, 2008.
3. D. H. Bernstein, E. Giladi, K. R. W. Jones, Eigenstates of the gravitational schrödinger equation. *Modern Physics Letters A* **13** (1998), no. 29, 2327–2336.
4. N. I. Danilina, N. S. Dubrovskaya, O. P. Kvasha, G. L. Smirnov, *Computational Mathematics*. Translated from the Russian by Irene Aleksanova. Mir, Moscow, 1988.
5. T. Graen, H. Grubmüller, NuSol–Numerical solver for the 3D stationary nuclear Schrödinger equation. *Computer Physics Communications* **198** (2016), 169–178.
6. A. A. Gusev, L. Le Hai, O. Chuluunbaatar, V. Ulziibayar, S. I. Vinitsky, V. L. Derbov, A. Góźdź, V. A. Rostovtsev, Symbolic-numeric solution of boundary-value problems for the Schrödinger equation using the finite element method: scattering problem and resonance states. In: *Computer algebra in scientific computing*, 182–197, Lecture Notes in Comput. Sci., 9301, Springer, Cham, 2015.
7. R. Harrison, I. Moroz, K. P. Tod, A numerical study of the Schrödinger–Newton equation 1: Perturbing the spherically-symmetric stationary states. *Preprint* 2002. `https://arxiv.org/abs/math-ph/0208045`.
8. V. I. Krylov, V. V. Bobkov, P. I. Monastyrnyĭ, *Numerical Methods*, vol. I. (Russian) Izdat. Nauka, Moscow, 1976.
9. C. Lanczos, An iteration method for the solution of the eigenvalue problem of linear differential and integral operators. *J. Research Nat. Bur. Standards* **45** (1950), 255–282.
10. Sh. Li, Z. Zhang, Computing eigenvalues and eigenfunctions of Schrödinger equations using a model reduction approach. *Commun. Comput. Phys.* **24** (2018), no. 4, 1073–1100.
11. A. A. Samarskiĭ, *Introduction to the Theory of Difference Schemes*. (Russian) Izdat. Nauka, Moscow, 1971.
12. P. Sandin, M. Örgen, M. Gullikson, Numerical solution of the stationary multicomponent nonlinear Schrödinger equation with a constraint on the angular momentum. *Phys. Rev. E* **93** (2016), no. 3, 033301, 7 pp.
13. A. Voros, Exact resolution method for general 1D polynomial Schrödinger equation. *J. Phys. A* **32** (1999), no. 32, 5993–6007. Corrigendum: *J. Phys. A* **33** (2000), no. 32, 5783–5784.

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