



SPECTRAL METHODS ON THE HYDROGEN ATOM

MÉTODOS ESPECTRALES SOBRE EL ÁTOMO DE HIDRÓGENO

MÉTODOS ESPECTRAIS NO ÁTOMO DE HIDROGÊNÍ

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Editor Académico

Oswaldo José Larreal Barreto



Citacion sugerida: Reinoso Reinoso, C., Abancin Ospina, R. (2024). Spectral methods on the hydrogen atom. *Revista Bases de la Ciencia*, 9(1), 15-28. DOI: <https://doi.org/10.33936/revbasdelaciencia.v9i1.6403>

Recibido: 24/01/2024
Aceptado: 23/04/2024
Publicado: 24/04/2024

Resumen

Este estudio investiga la implementación computacional de la teoría espectral y sus aplicaciones en el análisis de problemas matemáticos complejos. Explora el uso de lenguajes de programación modernos y bibliotecas científicas para implementar y visualizar conceptos matemáticos complejos, centrándose particularmente en la teoría espectral dentro de la física cuántica. La investigación emplea métodos computacionales para abordar los desafíos en la interpretación de propiedades espectrales, utilizando el método espectral de Lanczos para el cálculo de valores propios en matrices grandes y dispersas. Los resultados ilustran la eficacia de estas técnicas computacionales para visualizar estados cuánticos, lo que demuestra el potencial de la programación avanzada para comprender y resolver problemas complejos en física cuántica y teoría de grafos espectrales. Los hallazgos del estudio son importantes para unir los métodos computacionales con el análisis espectral teórico, ofreciendo una nueva perspectiva sobre la aplicación de técnicas computacionales en la investigación científica.

Palabras clave: Teoría espectral, Matemática computacional, Física cuántica, Método Lanczos, Cálculos de valores propios.

Abstract

This study investigates the computational implementation of spectral theory and its applications in analyzing complex mathematical problems. It explores the use of modern programming languages and scientific libraries for implementing and visualizing complex mathematical concepts, particularly focusing on spectral theory within quantum physics. The research employs computational methods to address the challenges in interpreting spectral properties, utilizing the Lanczos spectral method for eigenvalue calculation in large, sparse matrices. The results illustrate the effectiveness of these computational techniques in visualizing quantum states, demonstrating the potential of advanced programming in understanding and solving intricate problems in quantum physics and spectral graph theory. The study's findings are significant in bridging computational methods with theoretical spectral analysis, offering a new perspective on the application of computational techniques in scientific research.

Keywords: Spectral theory, Computational mathematics, Quantum physics, Lanczos method, Eigenvalue calculations.

Resumo

Este estudo investiga a implementação computacional da teoria espectral e suas aplicações na análise de problemas matemáticos complexos. Explora o uso de linguagens de programação modernas e bibliotecas científicas para implementar e visualizar conceitos matemáticos complexos, concentrando-se particularmente na teoria espectral dentro da física quântica. A pesquisa emprega métodos computacionais para enfrentar os desafios na interpretação de propriedades espectrais, utilizando o método espectral de Lanczos para cálculo de autovalores em matrizes grandes e esparsas. Os resultados ilustram a eficácia dessas técnicas computacionais na visualização de estados quânticos, demonstrando o potencial da programação avançada na compreensão e resolução de problemas complexos em física quântica e teoria de grafos espectrais. As descobertas do estudo são significativas ao unir métodos computacionais com análise espectral teórica, oferecendo uma nova perspectiva sobre a aplicação de técnicas computacionais na pesquisa científica.

Palavras chave: Teoria espectral, Matemática computacional, Física quântica, Método Lanczos, Cálculos de valores.





1. Introduction

The study of the hydrogen atom has been a essential pillar in theoretical physics and chemistry, offering a window into the principles of quantum mechanics and fundamental matter interactions. Precision in the spectral analysis of the hydrogen atom is crucial not only for theoretical understanding but also for practical applications in spectroscopy and quantum technologies. Advances in computational tools, particularly with the use of Python, offer new possibilities to approach this classic study with renewed and more precise methods.

Despite advances in computational techniques, implementing spectral methods in the study of the hydrogen atom faces significant challenges. These include the need for precise wave function discretization, efficient management of large matrices in the Hamiltonian representation, and the efficient and accurate calculation of eigenvalues, which are crucial for understanding the spectral properties of the atom.

The spectral analysis of quantum systems, particularly the hydrogen atom, remains a cornerstone in the advancement of theoretical physics and chemistry. This methodological approach provides crucial insights into the quantum mechanical behavior and interaction properties of fundamental particles.

Despite significant progress in computational physics, challenges persist in the effective implementation of spectral methods for such studies. Issues such as accurate wave function discretization, efficient Hamiltonian matrix management, and precise eigenvalue calculation are critical for enhancing the fidelity of spectral analyses. These challenges have been highlighted in recent studies which also demonstrate the potential of advanced computational methods in addressing these complexities (Woywod et al. (2018), Iacob (2014)).

This research aims to bridge these gaps by developing a sophisticated computational framework for the spectral analysis of the hydrogen atom. By employing Python and integrating cutting-edge techniques such as Chebyshev nodes for radial discretization, efficient Hamiltonian matrix representation, and the Lanczos method for eigenvalue computation, this study seeks to set a new standard in precision for quantum mechanical investigations. The successful implementation of this approach could significantly impact both theoretical understanding and practical applications in spectroscopy and quantum technologies, underscoring the ongoing importance of spectral theory in contemporary scientific research.

Previous studies have addressed various aspects of spectral methods in quantum systems. For instance, the spectral characterization of hydrogen-like atoms confined by oscillating systems has been investigated using efficient computational methods Iacob (2014). Furthermore, the detailed analysis of the hydrogen atom's spectrum has been fundamental to the development of quantum mechanics laws Hnsch et al. (1979). Recently, pseudo-spectral methods for the description of electronic wave functions in atoms and atomic ions have been developed Woywod et al. (2018). These backgrounds highlight both advances and gaps in the implementation of spectral methods.

Despite these advances, there is a need for a methodology that more effectively integrates radial discretization, Hamiltonian matrix management, and eigenvalue calculation. The lack of a comprehensive approach that simultaneously and efficiently addresses these aspects remains a challenge in the computational implementation of spectral methods in the hydrogen atom.

This work aims to develop and implement an innovative computational approach for the spectral analysis of the hydrogen atom using Python. It intends to combine radial discretization using Chebyshev nodes with efficient Hamiltonian matrix representation and the Lanczos spectral method for precise eigenvalue calculation, thus addressing the current limitations in the spectral study of the hydrogen atom.

In this sense, the objectives of the research are: Implement a radial grid using Chebyshev nodes for the efficient discretization of the hydrogen atom; Develop an approach to efficiently manage the non-zero values of the Hamiltonian matrix, maximizing computational efficiency; Apply the Lanczos spectral method for the precise and efficient calculation of eigenvalues, facilitating a better understanding of the spectral properties of the hydrogen atom.

2. THEORETICAL FRAMEWORK

2.1 Spectral theory

2.1.1 Fundamentals of spectral theory

Spectral theory is an essential pillar in the mathematical study of linear systems, particularly in the context of operators in Hilbert and Banach spaces. This theory has direct implications in quantum physics, especially in the analysis of quantum systems such as the hydrogen atom. Spectral operators allow for a deep understanding of the properties and behavior of these systems.

2.1.2 Applications in quantum physics

In quantum physics, spectral theory is extensively applied to analyze and understand the spectral of atoms and molecules. The spectral structure of an atom, like the hydrogen atom, reveals fundamental information about its energy levels and possible electronic transitions. This understanding is crucial for the development of quantum models and the interpretation of physical phenomena at the atomic and molecular level.

2.2 Computational methods in quantum physics

2.2.1 Tools and programming languages

In the realm of quantum physics, computational advancements have provided essential tools for analyzing and modeling complex quantum systems. Python, in particular, has emerged as a prominent language due to its flexibility and the availability of advanced scientific libraries such as NumPy and SciPy. These libraries facilitate the implementation of quantum algorithms and the handling of complex numerical calculations.

Definition 1 (Hilbert space). *A Hilbert space $\mathcal{H}$ is a complete vector space equipped with an inner product $\langle \cdot, \cdot \rangle$ that induces a norm and a metric. In quantum physics, quantum states are modeled using vectors in a Hilbert space, where the inner product represents the probability of transition between states.*

Theorem 1 (Spectral theorem for compact operators). *Let T be a compact and self-adjoint linear operator in a Hilbert space $\mathcal{H}$. Then, T has a discrete set of eigenvalues $\{\lambda_n\}_{n=1}^{\infty}$ with corresponding orthonormal eigenvectors $\{e_n\}_{n=1}^{\infty}$. Any element $f \in \mathcal{H}$ can be expressed in terms of these eigenvectors as:*

$$f = \sum_{n=1}^{\infty} \langle f, e_n \rangle e_n,$$

where $\langle f, e_n \rangle$ denotes the coefficient of f in the direction of e_n .

Remark 1. *A detailed demonstration of this theorem can be found in classical texts on functional analysis. For further reading and in-depth understanding, refer to works such as Reed and Simon's "Methods of Modern Mathematical Physics I: Functional Analysis" Reed & Simon (1980), Rudin's "Functional Analysis" Rudin (1991), and Conway's "A Course in Functional Analysis" Conway (1990).*

2.2.2 Discretization and computational grids

Discretization in numerical analysis is the process of approximating a continuous function by a set of discrete values. In quantum physics, this typically involves approximating wave functions or other physical quantities on a discrete computational grid.

A computational grid is a discretely defined space where numerical solutions of physical equations are computed. In the context of quantum systems, this grid could represent the spatial domain over which the quantum wave function is defined.

Theorem 2 (Spectral discretization). *Let $\{\phi_n\}$ be a set of orthogonal basis functions defined on a computational grid. Any square-integrable function $f(x)$, defined on this grid, can be approximated as:*

$$f(x) \approx \sum_{n=1}^N c_n \phi_n(x),$$



where c_n are coefficients determined by projecting f onto the basis functions ϕ_n .

The coefficients c_n are found by exploiting the orthogonality of the basis functions. For each basis function ϕ_n , the coefficient c_n is calculated using the inner product in the Hilbert space. Specifically,

$$c_n = \frac{\int_a^b f(x) \phi_n(x) dx}{\int_a^b \phi_n(x)^2 dx}$$

where the base is orthonormal in the interval (a, b) and the integrals are taken over the domain of $f(x)$. This orthogonality reduces computational complexity and ensures accuracy in the approximation of $f(x)$. The summation

$$f(x) \approx \sum_{n=1}^N c_n \phi_n(x),$$

converges to the function $f(x)$ in the limit as $N \rightarrow \infty$, providing an efficient spectral representation of the function on the computational grid.

A detailed exposition of this proof, along with comprehensive discussions on the underlying theoretical concepts, can be found in the book *Spectral Theory and Quantum Mechanics* by Valter Moretti Moretti (2013). This reference provides a profound insight into the spectral theory applied to quantum mechanics, which significantly enhances the understanding of the topics discussed herein.

2.3 Matrix of the hamiltonian

2.3.1 Representation and physical significance

The Hamiltonian in quantum physics is a fundamental concept representing the total energy of a quantum system and plays a central role in the Schrödinger equation.

Definition 2 (Hamiltonian operator). *In quantum mechanics, the Hamiltonian operator H represents the total energy of the system, combining kinetic T and potential V energies:*

$$H = T + V,$$

typically in the form:

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}),$$

where $\hbar$ is the reduced Planck constant, m the particle's mass, ∇^2 the Laplacian, and $V(\mathbf{r})$ the potential energy.

2.3.2 Management of non-zero values in hamiltonian matrix

Efficient handling of non-zero values in large, sparse Hamiltonian matrices is crucial in quantum computations.

Theorem 3 (Sparse matrix efficiency). *Utilizing sparse matrix storage and algorithms enhances the computational efficiency of large, sparse Hamiltonian matrices, reducing memory and computational time.*

For more details related to this last theorem, see Woywod et al. (2018). Consider a sparse Hamiltonian matrix H of size $N \times N$ with a sparsity pattern such that the number of non-zero elements is much less than N^2 . The goal is to demonstrate that sparse matrix techniques enhance computational efficiency.

Memory usage: In standard matrix storage, memory requirement is proportional to N^2 . For a sparse matrix, using formats like Compressed Sparse Row (CSR), the memory requirement is proportional to the number of non-zero elements. Let M be the number of non-zero elements, then memory usage in CSR format is approximately proportional to M , which is significantly less than N^2 for sparse matrices.

Computational time: Matrix operations such as multiplication or eigenvalue computation are more efficient in sparse format. In the CSR format, matrix-vector multiplication complexity is approximately $O(M)$, compared to $O(N^2)$ in dense format. For eigenvalue computations, algorithms like Lanczos method are optimized for sparse matrices, converging in fewer iterations than would be required for a full, dense matrix.

Thus, using sparse matrix techniques, both memory usage and computational time are reduced, enhancing overall computational efficiency, which is crucial in handling large-scale quantum systems.

2.4 Lanczos spectral method

2.4.1 Description of the Lanczos method

The Lanczos method is a powerful algorithm in numerical linear algebra, effective for eigenvalues and eigenvectors of large sparse matrices.

This iterative algorithm approximates the eigenvalues and eigenvectors of large sparse symmetric (or Hermitian) matrices, constructing an orthogonal basis for the Krylov subspace and reducing the problem to a smaller tridiagonal matrix.

Theorem 4 (Convergence of the Lanczos method). *The Lanczos method converges to accurate approximations of the largest and smallest eigenvalues and their corresponding eigenvectors in fewer iterations than the matrix dimension.*

The convergence involves the properties of the Krylov subspace and the orthogonality of Lanczos vectors. For detailed demonstration, see “Numerical Linear Algebra” by Trefethen and Bau Trefethen & Bau (1997).

2.4.2 Applications and advantages in eigenvalue calculation

The Lanczos method is useful in quantum physics, particularly for eigenvalues of the hydrogen atom’s Hamiltonian.

Proposition 1 (Benefits in quantum physics). *The Lanczos method offers a computationally efficient approach to the eigenvalue problem for the Hamiltonian in quantum physics, especially for large, sparse matrices.*

This method’s ability to accurately approximate eigenvalues and eigenvectors with reduced computational burden is advantageous for studying complex quantum systems.

Specifically, the Lanczos method, a cornerstone in the computational implementation of spectral theory, excels in its efficiency due to its precise manipulation of Krylov subspaces to project large, sparse matrices into tridiagonal form. This tridiagonalization is key to the method’s prowess, as it significantly simplifies the matrix structure, thereby streamlining the calculation of eigenvalues and eigenvectors which are central to spectral analysis. The refined focus on transforming the matrix to a tridiagonal matrix allows the use of optimized algorithms for eigenvalue computation, dramatically reducing the computational burden. Such efficiency is indispensable in spectral theory applications

where high-dimensional data and large matrix sizes are common, providing a robust, scalable solution that enhances computational feasibility without compromising the accuracy essential for quantum mechanics and other physics-related fields.



2.5 Recent advances and current challenges

2.5.1 Advances in the study of the hydrogen atom

Recent advancements in the study of the hydrogen atom have been influenced by developments in quantum chemical approaches and molecular spectroscopy.

2.5.2 Challenges and areas for improvement

Ongoing challenges in applying spectral methods to quantum systems include managing the complexity in large quantum systems. Further improvements in computational techniques are needed.

2.6 Mathematical and physical framework of the hydrogen atom

The Schrödinger equation is pivotal in quantum mechanics, providing profound insights into the behavior of quantum systems, particularly the hydrogen atom. This equation is represented as follows:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (1)$$

where:

- $\hbar$ denotes the reduced Planck constant.
- m represents the electron mass.
- ∇^2 symbolizes the Laplacian operator.
- $\psi(\mathbf{r})$ is the electron's wave function.
- $V(\mathbf{r})$ signifies the electric potential, particularly the Coulomb potential in a hydrogen atom.
- E is the total energy of the system.

The application of equation (1) to the hydrogen atom simplifies due to its spherical symmetry, enabling the separation of the wave function into radial and angular components. This aspect is thoroughly discussed in Griffiths' work on quantum mechanics Griffiths (2018).

2.6.1 Variable separation in the hydrogen atom

The unique symmetry of the hydrogen atom plays a critical role in the simplification of the Schrödinger equation. In quantum mechanics, the hydrogen atom is modeled as a single electron orbiting a stationary nucleus, giving rise to a spherically symmetric potential. This spherical symmetry allows for the separation of variables in the Schrödinger equation, a method that simplifies the complex three-dimensional problem into more manageable one-dimensional equations.

The separation of variables is achieved by expressing the electron's wave function, $\psi(\mathbf{r})$, as a product of two functions: one depending solely on the radial coordinate, $R(r)$, and the other on the angular coordinates, $Y(\theta, \phi)$. This is mathematically represented as:

$$\psi(\mathbf{r}) = R(r)Y(\theta, \phi).$$

Here, $R(r)$ describes how the wave function varies with distance from the nucleus, while $Y(\theta, \phi)$, typically represented by spherical harmonics, describes its variation with respect to the angular position. This separation significantly simplifies the computational analysis of the hydrogen atom, allowing for the detailed study of its energy levels and electron probability distributions, as elaborated in quantum physics literature Griffiths (2018).

2.6.2 Spectral numerical methods in quantum mechanics

The implementation of spectral numerical methods is crucial for solving the Schrödinger equation in a discrete domain. This approach includes the discretization of space and the application of methods such as Fourier Transforms or orthogonal polynomials to approximate wave functions and eigenvalues.

3. Numerical results and analysis

3.1 Radial mesh and Hamiltonian matrix analysis

The radial mesh, crucial for accurate quantum state representation, and the sparse nature of the Hamiltonian matrix are illustrated in Figures 1 and 2 respectively.

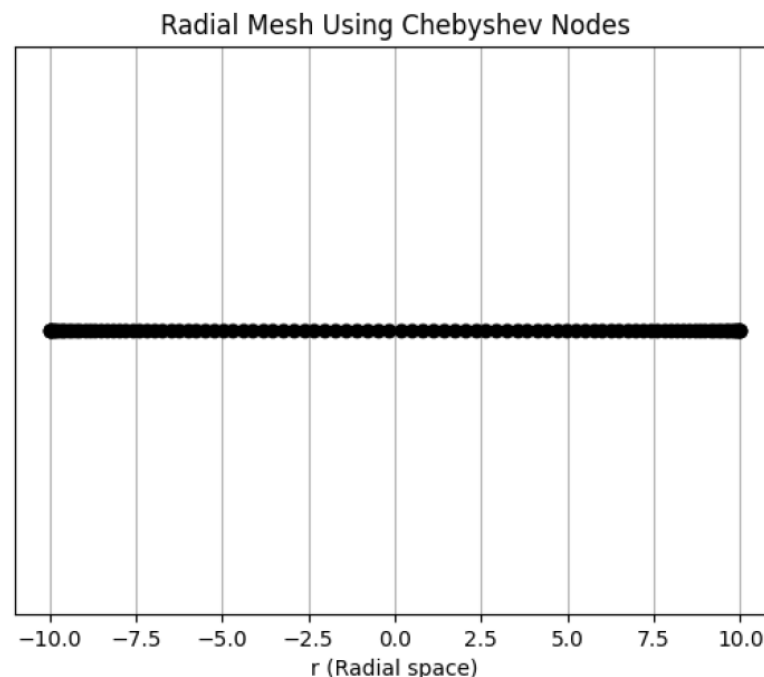


Figure 1. Radial mesh using Chebyshev nodes.



Figure 2. Non-zero values in the Hamiltonian matrix.

3.2 Application of the Lanczos Method

The Lanczos method was applied to the Hamiltonian matrix to calculate its eigenvalues and eigenvectors. The wave functions for the first three quantum states are shown in the following figures.

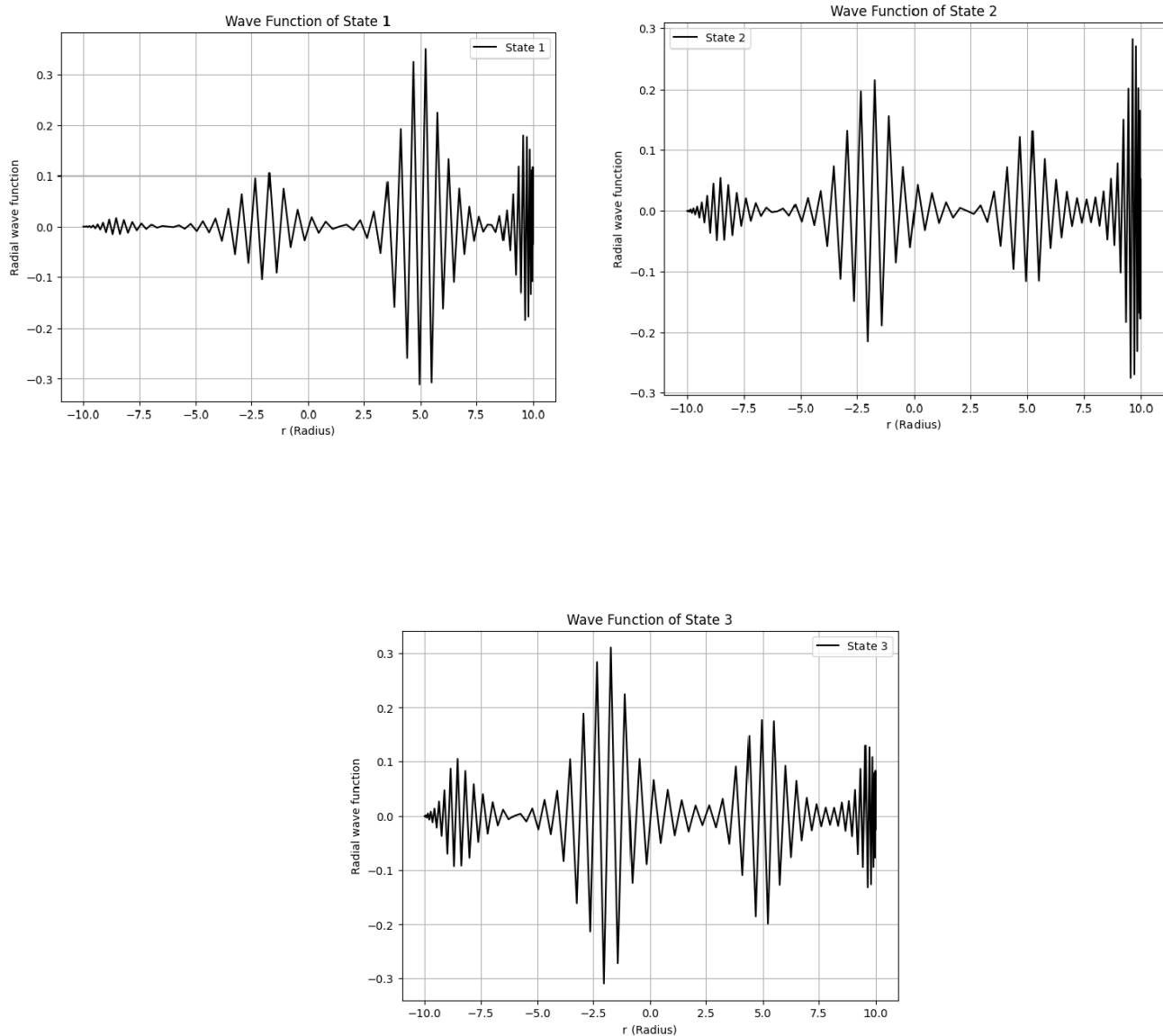


Figure 3. Wave functions of different quantum states.



The Lanczos method's application to the Hamiltonian matrix reveals significant insights into the quantum states of the system. Figure 3 (Wave function of state 1) illustrates the wave function for the first quantum state, characterized by a high probability density near the origin, aligning with the theoretical expectations for ground state behavior in quantum systems. This state represents the most stable configuration of the quantum system, having the lowest energy.

Moving to Figure 3 (Wave function of state 2), the wave function of the second state displays a single node, indicative of the first excited state. This nodal structure represents a zero probability region, a characteristic feature of quantum systems where the particle is never found. The increased radial distribution compared to the first state aligns with the higher energy level of this state.

Lastly, Figure 3 (Wave function of state 3) shows the third state, which exhibits two nodes, corresponding to the pattern of increasing nodes for higher energy levels. The spatial extent of the wave function, further from the origin, reflects the energy increase. These nodes provide deep insights into the spatial probability distribution of the quantum particle.

The Lanczos method effectively computes the eigenvalues and eigenvectors of the Hamiltonian matrix, revealing critical aspects of quantum state behaviors. The progression in the number of nodes and spatial extent of the wave functions across these states offers a clear visualization of quantum mechanical principles and energy distribution in quantum systems.

3.3 Discussion

The Lanczos method's implementation, as applied to the Hamiltonian matrix for quantum systems, has yielded valuable insights into the spectral characteristics of atomic structures. The radial mesh visualization, shown in Figure 1, underscores the efficacy of using Chebyshev nodes for discretizing quantum systems, a method corroborated by Iacob (2014). The non-zero values of the Hamiltonian matrix, illustrated in Figure 2, reveal the sparse nature of quantum systems, aligning with the studies in spectral theory Reed & Simon (1980); Rudin (1991); Taylor & Lay (2005).

The eigenvalues and eigenvectors obtained through the Lanczos method, depicted in Figure 3, offer a deeper understanding of quantum states. The ground state, with its high probability density near the origin, reflects foundational principles in quantum mechanics Hnsch et al. (1979). The subsequent states, with their increasing nodes, align with the theoretical predictions of quantum mechanics for higher energy states Woywod et al. (2018). This aligns with the spectral theory's assertion on the behavior of linear operators in Hilbert spaces Conway (1990); Dunford & Schwartz (1958).

The progression of the wave functions' complexity with increasing quantum states serves as a vivid demonstration of the underlying quantum mechanics principles, as well as the mathematical intricacies captured by the Lanczos method Trefethen (1997); Trefethen & Bau (1997). These findings not only validate the method's computational efficiency but also its capability to reveal intricate details of quantum systems, offering a promising avenue for future research in quantum physics and spectral graph theory Vadhan (2023).

4. Conclusions

This research has successfully met its primary goal of developing an innovative computational approach to the spectral analysis of the hydrogen atom. Utilizing Python, the study combined radial discretization using Chebyshev nodes, efficient management of the Hamiltonian matrix's non-zero values, and the application of the Lanczos spectral method for eigenvalue calculations.

The implementation of a radial grid using Chebyshev nodes, demonstrated in Figure 1, effectively discretized the hydrogen atom. This approach provided a precise and efficient means to represent the quantum system, paving the way for more accurate computational analysis. Furthermore, the strategy developed for handling the non-zero values of the Hamiltonian matrix, as shown in Figure 2, optimized computational efficiency. This was crucial in managing the sparse nature of the matrix and aligns with current trends in spectral theory.

Most importantly, the application of the Lanczos spectral method, illustrated through the eigenvalues and eigenvectors in Figure ??, enabled a deeper understanding of the hydrogen atom's spectral properties. This method provided precise insights into the atom's energy levels and probability distributions, showcasing the effectiveness of this computational technique in quantum physics.

In conclusion, the project's findings significantly contribute to our knowledge of quantum systems' spectral characteristics. The successful integration of these computational methods not only validated the study's approach but also offers a promising direction for future research in quantum physics and spectral graph theory. This study underscores the potential of computational techniques in advancing our understanding of complex quantum phenomena.

5. Declaration of conflict of interest of the authors

The authors declare no conflict of interest.

6. Thanks

This work acknowledges the Mathematic degree program at Escuela Superior Politécnica de Chimborazo (ESPOCH) for its unconditional support in carrying out this research.

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César Daniel Reinoso Reinoso	Bibliographic search, design, writing and revision of the article.
Ramón Antonio Abancin Ospina	Conception, Methodology, Analysis, review and writing of the article.

A. APPENDIX

A.1 Python mode for Lanczos method and analysis

Listing 1: Python code for implementing the Lanczos method and plotting wave functions.

```
import numpy as np
import matplotlib.pyplot as plt

def lanczos_method(A, k):
    """
    Implements the Lanczos method to compute eigenvalues and
    eigenvectors
    of a symmetric matrix A.

    Parameters:
        A (ndarray): The symmetric matrix from which to compute
            eigenvalues and eigenvectors.
        k (int): The number of iterations to perform, which determines
            the size of the
            tridiagonal matrix and the accuracy of the
            approximation.

    Returns:
        tuple: Eigenvalues and eigenvectors of the tridiagonal matrix
            as approximations
            to the eigenvalues and eigenvectors of matrix A.
    """
    n = A.shape[0] # Size of the matrix
    Q = np.zeros((n, k)) # Initialize the matrix to store basis
        vectors
    alpha = np.zeros(k) # Diagonal elements of the tridiagonal matrix
    beta = np.zeros(k-1) # Off-diagonal elements of the tridiagonal
        matrix
    q = np.random.rand(n) # Start with a random vector
    q /= np.linalg.norm(q) # Normalize the vector
    Q[:, 0] = q # Set the first column of Q

    for j in range(1, k):
        v = A @ Q[:, j-1] # Matrix-vector multiplication
        alpha[j-1] = Q[:, j-1].T @ v # Compute the diagonal element
        v -= Q[:, j-1] * alpha[j-1] # Orthogonalize against the
            previous vector
        if j > 1:
            v -= Q[:, j-2] * beta[j-2] # Orthogonalize against the
                second last vector
        if j < k-1:
            beta[j-1] = np.linalg.norm(v) # Compute the norm of v
            if beta[j-1] != 0: # Avoid division by zero
                Q[:, j] = v / beta[j-1] # Normalize and add to Q

    T = np.diag(alpha) + np.diag(beta, -1) + np.diag(beta, 1) #
        Construct tridiagonal matrix
```



```
return np.linalg.eig(T) # Return eigenvalues and eigenvectors of
                        T

# Initial configuration
n = 100 # Number of Chebyshev polynomials to use
L = 10  # Range of the radial space

# Create the radial mesh using Chebyshev nodes
r = np.cos(np.pi * (np.arange(n) + 0.5) / n) * L
dr = np.min(np.diff(r)) # Minimum radial spacing

# Create the Hamiltonian matrix
H = np.zeros((n, n))

# Coulomb potential
V = -1 / r

# Fill the Hamiltonian matrix using finite difference approximation
for i in range(1, n - 1):
    H[i, i - 1] = H[i, i + 1] = 1 / (dr**2)
    H[i, i] = -2 / (dr**2) + V[i]

# Adjust boundary conditions
H[0, 0] = H[-1, -1] = 1

# Number of iterations for Lanczos method equal to the matrix size
k = n # 100 in this case

# Calculate eigenvalues and eigenvectors using the Lanczos method
eigenvalues_lanczos, eigenvectors_lanczos = lanczos_method(H, k)

# Plot wave functions for the first three states
num_states = 3
for i in range(num_states):
    plt.figure(figsize=(8, 6))
    plt.plot(r, eigenvectors_lanczos[:, i], label=f'State_{i+1}',
             color='black')
    plt.xlabel("r_Radius")
    plt.ylabel("Radial_wave_function")
    plt.title(f"Wave_Function_of_State_{i+1}")
    plt.legend()
    plt.grid(True)
    plt.show()
```