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On computation for a hydrogen atom in arbitrary magnetic fields using finite volume method

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Abstract. The Schrödinger equation in a 2D cylindrical coordinate system is numerically solved for the ground state and a few excited states of the hydrogen atom in arbitrary magnetic fields. The second order discretization of the PDEs on finite volumes results in a set of algebraic equations that are solved simultaneously using Gauss-Seidel Algebraic Multi-Grid (AMG) solver. The modified Stodola-Vianello method is implemented using Gram-Schmidt orthogonalization process to extract the first few energy states and their wave functions concurrently. A detailed mesh convergence study suggests that both energies and wave functions correctly approach toward the unknown exact solutions.

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Key words: Schrödinger equation, hydrogen atom, magnetic field, finite volume method, eigenvalues, eigenvectors

1 Introduction

The problem of hydrogen atoms in magnetic fields of arbitrary strength is of great relevance in astrophysics, atomic and molecular physics, and certain areas of solid-state physics. The Schrödinger equation for a hydrogen atom in a magnetic field is inseparable and unsolvable analytically due to spherical symmetry of Coulomb potential and cylindrical symmetry of magnetic potential. In the absence of a closed form solution, many numerical methods have been adopted to establish high precision energy spectrum of hydrogen atom over a wide range of magnetic strength. There is not much known about the structure of a hydrogen atom with a magnetic field in terms of wave functions. Most approaches use certain wave function expansions or approximations for estimating energy spectrum. Perturbation theory is well suited for weak-field regime [1,2] while adiabatic

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approximation is for very strong-field regime [3,4]. Rösner *et al*. [5] computed the high precision energy spectrum over a wide range of magnetic fields using Hartee-Fock-like methods [6]. The method seemed to perform poorly in the intermediate field region due to competing Coulomb and magnetic forces. A few successful variational calculations have also been reported in [7,8]. Kravchenko *et al*. [9] has provided some outline of exact solutions to this problem in forms of the power series in the radial variable and through the sine of the polar angle. Different numerical methods for the hydrogen atom in a magnetic field have been reported by many authors [10-16], and high precision energy spectrum of the hydrogen atom has been achieved. However, the literature lacks the detailed structure of hydrogen wave functions for low to very high magnetic fields. It is the purpose of this paper to compute both energies and wave functions that approximate toward the exact solutions through mesh convergence study by directly solving the Schrödinger equation numerically for the first few energy states over a wide range of magnetic fields.

2 Finite volume formulation and solution procedure

The time-independent Schrödinger equation in a 2D cylindrical coordinate system (ρ, z) using atomic units for a hydrogen atom (spin down) with a uniform magnetic field aligned with z-axis can be written as

$$\begin{aligned} &-\frac{1}{2}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right)+\frac{\partial^2\psi}{\partial z^2}-\frac{m^2}{\rho^2}\psi\right] \\ &+\left(\frac{\gamma}{2}(m+2s_z)+\frac{\gamma^2\rho^2}{8}-\frac{1}{\sqrt{\rho^2+z^2}}\right)\psi=E\psi, \end{aligned} \tag{1}$$

where m is the magnetic quantum number and the magnetic field strength is $\gamma = B/B_0$, where $B_0 = 2.3505\times10^5$ T. The energy E is measured in atomic units. The symbol s_z is the spin z-projection, i.e. $s_z = -1/2$ in this analysis. Since we adopt an iterative procedure for the first few modes, let the superscript n+1 stands for current iteration value, superscript n for previous iteration value, and the subscript i for the i^{th} mode. For a given m, if i=1,2,3….N modes, there will be N partial differential equations to be solved simultaneously. If the potential V is denoted as

$$V=\left(\frac{m^2}{2\rho^2}+\frac{\gamma}{2}(m-1)+\frac{\gamma^2\rho^2}{8}-\frac{1}{\sqrt{\rho^2+z^2}}\right), \tag{2}$$

Eq. (1) can be written as

$$\begin{aligned} &-\frac{1}{2}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi_i^{n+1}}{\partial\rho}\right)+\frac{\partial^2\psi_i^{n+1}}{\partial z^2}\right] \\ &+(V^+\psi_i^{n+1}+V^-\psi_i^n)+\frac{(\psi_i^{n+1}-\psi_i^n)}{\Delta t}=E_i^n\psi_i^n. \end{aligned} \tag{3}$$