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COMPRESSED HYDROGEN ATOM UNDER DEBYE SCREENING IN STRONG MAGNETIC FIELD

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Abstract. Effect of high pressure and magnetic field on H atom in the atmosphere of magnetic white dwarfs is important subject in astrophysical investigations for understanding the physics of stellar interiors and diagnostic determination of astrophysical plasmas. The model of compressed H atom, centrally confined by impenetrable spherical box with proton-electron interaction given by Debye-Hückel potential, is the subject of this work. Energy levels of the model are obtained numerically solving the Schrödinger equation by Lagrange-mesh method and their variations with radius of the confining spherical box, screening parameter and magnetic field strength are discussed.

1. INTRODUCTION

Investigations of atomic properties in strong magnetic fields is of significant interest for astrophysics. Stimulus to this area of research came from the discovery of very strong magnetic fields in and in vicinity of compact astrophysical objects, such as white dwarf stars and neutron stars (see, e.g. Kemp et al. 1970). Field strengths for white dwarfs are of order $B \approx \left(10^2 - 10^5\right)$ T, and at the surface of some neutron stars magnetic field strength can be of order $B \approx 10^8$T.

These compact stars play the roles of natural physical laboratories for studying the properties of matter under extreme physical conditions. The extreme conditions imply not only huge field, but also presence of dense plasma (electron density can exceed 10^{23}cm^{-3}), high pressure and high temperature (neutron stars atmospheres are hot with temperature of order $\left(10^5 - 10^6\right)$ K). In order to study interaction between the atom and plasma with such parameters, the model of compressed or confined atom is adopted (see, e.g. Saha et al. 2002, Varshni 2003, Bhattacharyya et al. 2008) and Coulomb interaction between the atomic electrons and nucleus is replaced with Debye potential.

2. THEORETICAL BACKGROUND

2. 1. MODEL

The hydrogen atom, embedded in dense plasma, is modelled by an atom confined at the center of impenetrable spherical box of radius R_0. Effect of plasma environment is mimicked through Debye potential. The non-relativistic Hamiltonian of the atom in external static magnetic field, directed along z axis, in atomic units ($\hbar = m_e = |e| = 1$) and in spherical coordinates is given by

$$H = T(r,\theta) + V(r) + mB + \frac{1}{2}B^2 r^2 \sin^2\theta \,, \tag{1}$$

where m is magnetic quantum number and magnetic field strength B is in units of $B_0 = 4.7 \cdot 10^5$T. Here

$$T(r,\theta) = -\frac{1}{2}\frac{\partial^2}{\partial r^2} - \frac{1}{2r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) , \tag{2}$$

$$V(r) = \begin{cases} -\frac{e^{-\mu r}}{r}, & r < R_0 \\ \infty, & r \geq R_0 \,, \end{cases} \tag{3}$$

where μ is screening or Debye parameter. It depends on temperature and number density of the plasma and one can simulate different plasma conditions from a given value of of μ. Only the ground state ($m = 0$) is considered here, so that paramagnetic term in (1) vanishes.

2. 2. LAGRANGE-MESH METHOD

Lagrange-mesh method is a variational method coupled with Gauss quadrature associated with the mesh. The basis functions $f_i(x)$ on interval $[a, b]$ are Lagrange functions satisfying the cardinality (or Lagrange) condition

$$f_i(x_j) = \frac{1}{\sqrt{w_i}}\delta_{ij} \,, \quad (i, j = 1,\, 2,\, \ldots\, N) \tag{4}$$

where x_i and w_i are the points and weights, appearing in Gauss quadrature formula

$$\int_a^b g(x)dx \approx \sum_{i=1}^{N} w_i g(x_i) \,. \tag{5}$$

The functions f_i are Gauss orthogonal

$$\int_a^b f_i(x)f_j(x)dx \approx \delta_{ij} \,. \tag{6}$$

The simplicity of the method is that it does not require any explicit evaluation, analytical or numerical, of matrix elements of the potential, but only the values of this potential at mesh points

$$\int_a^b f_i(x)V(x)f_j(x)dx \approx V(x_i)\,\delta_{ij} \,. \tag{7}$$

In order to numerically solve Schrödinger equation

$$H\psi(r,\theta) = E\psi(r,\theta) \tag{8}$$

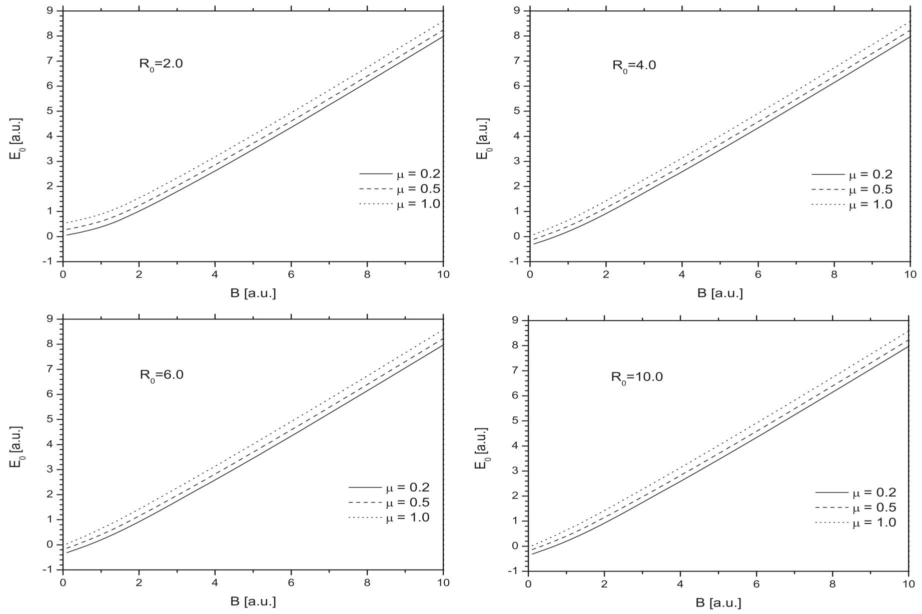

Figure 1: Variation of the ground state energy with magnetic field strength.

with Hamiltonian (1), it is required two-dimensional basis set with elements

$$F_{ij}(x,y) = f_i(x)g_j(y)\,, \tag{9}$$

where dimensionless coordinates $x = r/R_0$ and $y = \cos\theta$ ($0 \leq x \leq 1$, $-1 \leq y \leq 1$) were introduced. The problem is now reduced to eigenvalue problem of the Hamiltonian matrix with elements

$$H_{ij,kl} = \frac{1}{R_0^2}\left(T_x\right)_{ik}\delta_{jl} + \frac{1}{R_0^2 x^2}\left(T_y\right)_{jl}\delta_{ik} + V_{ij,kl}\left(x,y\right)\delta_{ik}\delta_{jl}\,, \tag{10}$$

where

$$T_x = -\frac{1}{2}\frac{d^2}{dx^2}\,,\quad T_y = -\frac{1}{2}\frac{d}{dy}\left(1-y^2\right)\frac{d}{dy}\,, \tag{11}$$

$$V(x,y) = -\frac{e^{-\mu R_0 x}}{R_0 x} + \frac{1}{2}B^2 R_0^2 x^2\left(1-y^2\right)\,. \tag{12}$$

The functions f_i ($i = 1, \ldots, N_x$) from (9) are Lagrange functions constructed from shifted Legendre polynomial of order N_x and regularized through multiplication by $x(1-x)$ in order to deal with singularity at the origin and to satisfy Dirichlet boundary condition at $x = 1$. The functions g_j ($i = 1, \ldots, N_y$) are constructed from Legendre polynomial of order N_y. The matrix elements of the operators in (11) can be found in literature (see, e.g. Baye 1995 and Baye & Sen 2008).

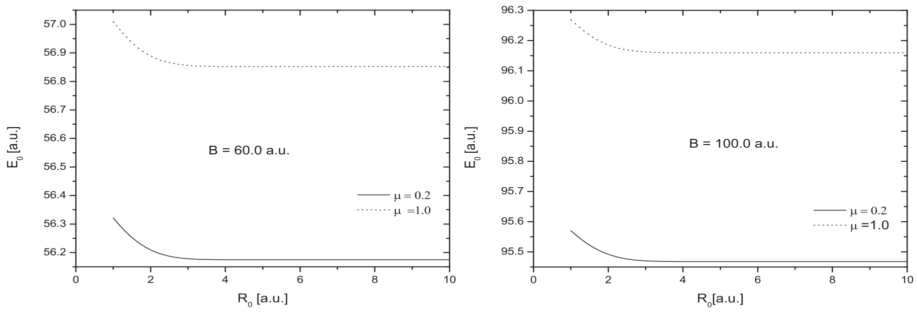

Figure 2: Variation of the ground state energy with the radius of confining sphere.

3. RESULTS AND DISCUSSION

The numerical method, described in the pervious section, is used to calculate ground state energy for different values of R_0, μ and B. Results are generated using the bases of different dimensions, from $N_x = 40$, $N_y = 50$ for lower values of B ($B \leq 10$) to $N_x = 80$, $N_y = 100$ for strong fields.

The ground state energy dependance on magnetic field strength from interval $(0.01 - 10.0)$ for different values of confining sphere radius and Debye parameter is displayed on figure 1. When R_0 and μ is fixed it is observed that energy increases with increasing in field strength. Moreover, when $R_0 > 2.0$ energy is negative for some or all the values of screening parameter μ, used here, for lower B values (up to $B \approx 1$) and positive for stronger fields. The behavior, described above, implies that for lower B values, confinement by the Debye potential dominates, and in stronger fields the confinement is caused by confining sphere and/or magnetic field.

When the magnetic field is stronger, i.e. when $B > 40.0$, and radius of confining sphere is $R_0 > 2.0$, the ground state energy is almost insensitive with increasing R_0 for given parameter μ. Figure 2 approves this statement. The cause for this type of behavior is confining effect of strong field magnetic field, which exceeds the confinement imposed by the spherical box.

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