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HYDROGEN ATOMS IN NEUTRON STAR ATMOSPHERES: ANALYTICAL APPROXIMATIONS FOR BINDING ENERGIES

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INTRODUCTION

Since the first observations of neutron stars thirty years ago, they have affected many branches of physics. These extremely compact stars serve as natural physical laboratories for probing the properties of matter under extreme physical conditions. In particular, more than half of them possess magnetic fields $B > 10^{12}$ G.

Despite their name, neutron stars consist not only of neutrons. They have a crust containing ionized iron, heavier elements, and exotic neutron-rich nuclei,[1] above which lie liquid and gaseous outer envelopes, which are thought to be composed of iron or lighter elements.[2] The atmosphere, that affects the spectrum of outgoing thermal radiation, likely consists of hydrogen, the most abundant element in the Universe, which might be brought to the star surface by fall-out of circumstellar medium. Neutral atoms can provide an appreciable contribution to the atmospheric opacity.

Apart from the physics of neutron stars, quantum-mechanical calculations of strongly magnetized hydrogen atoms find application also in the physics of white dwarf stars[3,4] and in the solid state physics.[5] Because of this practical demand, hydrogen in strong magnetic fields has been well studied in the past two decades.[6] The peculiarity of the problem for neutron stars is that an atom cannot be considered abstractedly from its thermal motion. Indeed, neutron star atmospheres are hot ($T \sim 10^5 - 10^6$ K), so that typical kinetic energies of the atoms are non-negligible in comparison with typical binding energies. Taking the thermal motion into account is highly non-trivial, because an atom moving across magnetic field is equivalent to an atom placed in orthogonal electric and magnetic fields, so that the cylindrical symmetry is broken.

At $\gamma \gg 1$, where $\gamma \equiv \hbar\omega_c/2 \text{ Ryd} = B/2.35 \times 10^9 \text{ G} \gg 1$ and ω_c is the electron cyclotron frequency, the collective motion effects[7,8] become especially pronounced. In particular, so-called decentered states (with the electron localized mostly in the "magnetic well" aside from the Coulomb center) are likely to be populated even at the relatively high densities $\rho > 10^{-2}$ g cm^{-3} typical of neutron star atmospheres. These exotic states have been predicted two decades ago by Burkova et al.[9] and studied recently by other authors.[10–12]

Collective-motion effects on the usual "centered" states have been first considered in frames of the theory of perturbation.[8,13] Non-perturbative results covering both centered and decentered states were subsequently presented for binding energies and

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wavefunctions,[14,15] oscillator strengths,[15] spectral line shapes,[16] and photoionization cross sections.[17] None of these data, however, has been published in an easy-to-use form of tables or analytical expressions.

In this contribution I propose approximate analytical expressions for the binding energies of the hydrogen atom arbitrarily moving in a magnetic field typical of neutron stars, $300 \le \gamma \le 10^4$. This range is physically distinguished, since at weaker fields the spectrum is strongly complicated by multiple narrow anticrossings,[14] while the upper bound, $\gamma \sim 10^4$, corresponds to the onset of non-negligible relativistic effects.[18]

THEORETICAL FRAMEWORK

Motion of the hydrogen atom in a magnetic field can be conveniently described by the pseudomomentum $\mathbf{K} = m_p\dot{\mathbf{r}}_p + m_e\dot{\mathbf{r}}_e - (e/c)\mathbf{B}\times(\mathbf{r}_e - \mathbf{r}_p)$, where the subscript $i = e$ or $i = p$ indicates electron or proton, respectively, $\dot{\mathbf{r}}_i = -(\mathrm{i}\hbar/m_i)\nabla_i - (q_i/m_i c)\mathbf{A}(\mathbf{r}_i)$ is the velocity operator, m_i the mass, $q_p = -q_e = e$ the charge, and $\mathbf{A}(\mathbf{r})$ the vector potential of the field. Gorkov and Dzyaloshinskii[19] have shown that in the representation in which all components of $\mathbf{K}$ have definite values, the relative motion can be described in terms of a one-particle Hamiltonian which depends on $\mathbf{K}$.

It is convenient to describe the centered states of the atom using the relative coordinate $\mathbf{r}^{(0)} = \mathbf{r}_e - \mathbf{r}_p$ as independent variable and the axial gauge of the vector potential, $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B}\times\mathbf{r}$. For the decentered states, the "shifted" representation[19] is more convenient. In the latter representation, the independent variable is $\mathbf{r}^{(1)} = \mathbf{r}_e - \mathbf{r}_p - \mathbf{r}_c$ and the gauge is $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B}\times(\mathbf{r} - [(m_p - m_e)/m_\mathrm{H}]\,\mathbf{r}_c)$. Here, $\mathbf{r}_c = \frac{c}{eB^2}\mathbf{B}\times\mathbf{K}$ is the relative guiding center, and $m_\mathrm{H} = m_p + m_e$.

Let us assume that $\mathbf{B}$ is directed along the z-axis. The z-component of the pseudomomentum corresponding to the motion along the field yields the familiar term $K_z^2/2m_\mathrm{H}$ in the energy, while the transverse components $\mathbf{K}_\perp$ produce non-trivial effects. Therefore we assume $K_z = 0$ and $\mathbf{K}_\perp = \mathbf{K}$ hereafter.

If there were no Coulomb attraction, then the transverse part of the wavefunction could be described by a Landau function $\Phi_{ns}(\mathbf{r}_\perp^{(1)})$, where $\mathbf{r}_\perp^{(1)}$ is the projection of $\mathbf{r}^{(1)}$ in the (xy)-plane. The energy of the transverse excitation is

$$E_{ns}^\perp = [n + (m_e/m_p)(n+s)]\hbar\omega_c, \tag{1}$$

where the zero-point and spin terms are disregarded.

A wavefunction ψ_κ of an atomic state $|\kappa\rangle$ can be expanded over the complete set of the Landau functions

$$\psi_\kappa^{(\eta)}(\mathbf{r}^{(\eta)}) = \sum_{ns} \Phi_{ns}(\mathbf{r}_\perp^{(\eta)})\, g_{n,s;\kappa}^{(\eta)}(z), \tag{2}$$

where $\eta = 0$ or 1 indicates the conventional or shifted representation, respectively (a generalization to arbitrary η proved to be less useful[15]). The one-dimensional functions $g_{ns;\kappa}^{(\eta)}$ are to be found numerically. The adiabatic approximation used in early works[9,19] corresponds to retaining only one term in this expansion.

A bound state can be numbered[15] as $|\kappa\rangle = |n_\kappa, s_\kappa, \nu, \mathbf{K}\rangle$, where n_κ and s_κ relate to the leading term of the expansion (2), and ν enumerates longitudinal energy levels

$$E_{n_\kappa,s_\kappa,\nu}^{\parallel}(K) = E_\kappa - E_{n_\kappa s_\kappa}^\perp \tag{3}$$

and controls the z-parity: $g_{n,s;\kappa}^{(\eta)}(-z) = (-1)^\nu g_{n,s;\kappa}^{(\eta)}(z)$. For the non-moving atom at $\gamma > 1$, the states $\nu = 0$ are tightly bound in the Coulomb well, while the states $\nu \ge 1$

Table 1. Parameters of the approximation (4) at $10^{-1} \le \gamma \le 10^4$.

s	0	1	2	3	4	5	6	7
p_1	15.55	0.5332	0.1707	0.07924	0.04696	0.03075	0.02142	0.01589
p_2	0.3780	2.100	4.150	6.110	7.640	8.642	9.286	9.376
p_3	2.727	3.277	3.838	4.906	5.787	6.669	7.421	8.087
p_4	0.3034	0.3092	0.2945	0.2748	0.2579	0.2431	0.2312	0.2209
p_5	0.4380	0.3784	0.3472	0.3157	0.2977	0.2843	0.2750	0.2682

are hydrogen-like, with binding energies below 1 Ryd. The states with $n \neq 0$ belong to continuum at $\gamma > 0.2$ and will not be considered here.

At small pseudomomenta K, the states $\nu = 0$ remain tightly bound and centered, the mean electron-proton separation $\bar{x}$ being considerably smaller than r_c (for the hydrogen-like states $\nu \ge 1$, however, $\bar{x}$ is close to r_c at any K). The larger K, the greater is the distortion of the wavefunction towards $\mathbf{r}_c$, caused by the motion-induced electric field in the co-moving reference frame, until near some K_c transition to the decentered state occurs, and the character of the motion totally changes. With further increasing K, the transverse velocity decreases and tends to zero, whereas the electron-proton separation increases and tends to r_c. Thus, for the decentered states, the pseudomomentum characterizes electron-proton separation rather than velocity.

At very large K the longitudinal functions become oscillator-like, corresponding to a wide, shallow parabolic potential well.[9] For a fixed ν, this limit is reached at $K \gg (\nu+\frac{1}{2})^2\hbar/a_\mathrm{B}$, where a_B is the Bohr radius. Still at arbitrarily large K, there remain infinite number of bound states with high values of ν whose longitudinal wavefunctions are governed by the Coulomb tail of the effective one-dimensional potential.[15]

The decentered states of the atom at $K > K_c \sim 10^2$ au have relatively low binding energies and large quantum-mechanical sizes, $l \sim K/\gamma$ au; therefore they are expected to be destroyed by collisions with surrounding particles in the laboratory and in the white-dwarf atmospheres. In neutron-star atmospheres at $\gamma \sim 10^3$, however, the decentered states may be significantly populated. This necessitates inclusion of the entire range of K below and above K_c in the consideration.

ANALYTICAL APPROXIMATIONS

Binding Energies of the Non-Moving Hydrogen Atom

Extensive tables of binding energies of the hydrogen atom at rest with respect to the magnetic field have been presented by Rösner et al.[20] and supplemented by other authors.[21–23] Recently, the accuracy $\sim 10^{-12}$ Ryd has been achieved.[24] In the astrophysics, a lower accuracy is usually sufficient, and simple analytical estimates are often desirable.

For this reason, we have constructed a fit to $E^{(0)}$, where $E^{(0)}_{ns\nu} \equiv -E^{\parallel}_{ns\nu}(0)$, in a possibly widest range of γ. For the tightly-bound states, we have

$$E^{(0)}_{0s0}(\gamma) = \ln\left(\exp\left[(1+s)^{-2}\right] + p_1\left[\ln(1+p_2\sqrt{\gamma})\right]^2\right) + p_3\left[\ln(1+p_4\gamma^{p_5})\right]^2 \text{ Ryd}. \quad (4)$$

The parameters $p_1 - p_5$ depend on s; they are listed in table 1. This fit is accurate to within 0.1–1% at $\gamma = 10^{-1} - 10^4$, and it also provides the correct limits at $\gamma \to 0$.

For the hydrogen-like states, we use the asymptotic result[25]

$$E^{(0)}_{ns\nu} = \frac{1\text{ Ryd}}{(N+\delta)^2}, \text{ where } \begin{cases} N = (\nu+1)/2, & \delta \sim \gamma^{-1} \quad \text{for odd } \nu, \\ N = \nu/2, & \delta \sim (\ln\gamma)^{-1} \quad \text{for even } \nu. \end{cases} \quad (5)$$

Table 2. Parameters of (5) at $1 \le \gamma \le 10^4$.

ν	1	2	3	4	5	6
a_ν	0.785	0.578	0.901	0.631	0.970	0.660
b_ν	1.724	0.765	1.847	0.717	1.866	0.693

We have obtained the following fits to the quantum defect δ: for odd ν, $\delta = (a_\nu + b_\nu\sqrt{\gamma} + 0.077\gamma)^{-1}$, where $a_\nu \approx 1$ and $b_\nu \approx 2$; and for even ν, $\delta = [a_\nu + 1.28\,\ln(1 + b_\nu\gamma^{1/3})]^{-1}$, where $a_\nu \approx \frac{2}{3}$ and $b_\nu \approx \frac{2}{3}$. More accurate values of a_ν and b_ν are given in table 2. At $1 \le \gamma \le 10^4$, errors of these approximations lie within $\sim 10^{-3}$.

Binding Energies of the Moving Hydrogen Atom

For the moving hydrogen atom in a strong magnetic field, the first analytical fit to $E(K)$ has been published by Lai and Salpeter.[26] It is rather accurate for the ground state at $K < K_c$ but cannot be applied to excited or decentered states.

We describe the longitudinal energy (3) by the formula

$$|E^{\parallel}_{ns\nu}(K)| = \frac{E^{(1)}_{ns\nu}(K)}{1 + (K/K_c)^{1/\alpha}} + \frac{E^{(2)}_{ns\nu}(K)}{1 + (K_c/K)^{1/\alpha}}. \qquad (6)$$

The two-term structure of (6) is dictated by the necessity to describe the two physically distinct regions of K below and above K_c. The parameter α has the meaning of the width of the transition region near K_c in logarithmic scale of pseudomomenta.

For the tightly-bound states, we parameterize the dependencies $E^{(j)}(K)$ as follows:

$$E^{(1)}_{0s0}(K) = E^{(0)}_{0s0} - \frac{K^2}{2m_{\rm eff} + q_1K^2/E^{(0)}_{0s0}}, \qquad E^{(2)}_{0s0}(K) = \frac{2\ \text{Ryd}}{\sqrt{r_*^2 + r_*^{3/2} + q_2 r_*}}, \qquad (7)$$

where $r_* = r_c/a_{\rm B} = K/(\gamma\ \text{au})$, q_1 and q_2 are dimensionless fitting parameters, and $m_{\rm eff}$ is the effective mass which is close to (but not necessarily coincident with) the transverse effective mass $M^{\perp}_{ns\nu}$ obtained by the perturbation technique. At $\gamma \ge 300$, we put $q_1 = \log_{10}(\gamma/300)$ if $s = 0$ and $q_1 = 0.5$ otherwise, $q_2 = 0.158\,[\ln((1+0.1s)\gamma/215)]^{2/5}$, and $\alpha = 0.053\,\ln(\gamma/150)$. For the effective mass, we have $m_{\rm eff} = m_{\rm H}\,[1 + (\gamma/\gamma_0)^{c_0}]$, where $c_0 = 0.937 + 0.038s^{1.58}$ and $\gamma_0 = 6150(1+0.0389s^{3/2})/[1+7.87s^{3/2}]$. For the critical pseudomomentum, we have $K_c = [c_1 + \ln(1 + \gamma/\gamma_1)]\sqrt{2m_{\rm H}E^{(0)}}$. The parameters c_1 and γ_1 take on the values $c_1 = 0.81, 1.09, 1.18, 1.24$ and $\gamma_1 = (8.0, 3.25, 2.22, 1.25) \times 10^4$ for $s = 0, 1, 2, 3$, respectively. For $s \ge 4$, we put $c_1 = 0.93 + 0.08s$ and $\gamma_1 = 6500$.

In figure 1 the above fitting formulae are compared with our numerical results[15] and with the previous approximations.[26] The figure demonstrates that the present approximations are valid at any K from 0 to infinity. Appreciable discrepancies occur only in narrow ranges of K near anticrossings.

Now let us turn to the hydrogen-like states. Their binding energies are approximated by the same formula (6) but with slightly different expressions for $E^{(1)}$ and $E^{(2)}$. For these states, $M^{\perp}_{ns\nu}$ exceeds $m_{\rm H}$ by orders of magnitude, and the perturbation method fails already at small K,[13] rendering the notion of the effective mass practically useless for the fitting. Thus we consider $m_{\rm eff}$ as effectively infinite and put $E^{(1)}_{0s\nu}(K) = E^{(0)}_{0s\nu}$ ($\nu \ge 1$). Furthermore, the transition region is not well defined, and therefore K_c and α lose their clear meaning and become mere fitting parameters. For odd states, we have, approximately, $K_c = (\nu^{5/4}\gamma/170)^{0.9}\sqrt{2m_{\rm H}E^{(0)}}$ and $\alpha = 0.66 + \nu/20$. For even states, $K_c = \nu\sqrt{(\gamma/600)m_{\rm H}E^{(0)}}$ and $\alpha = 0.66$.

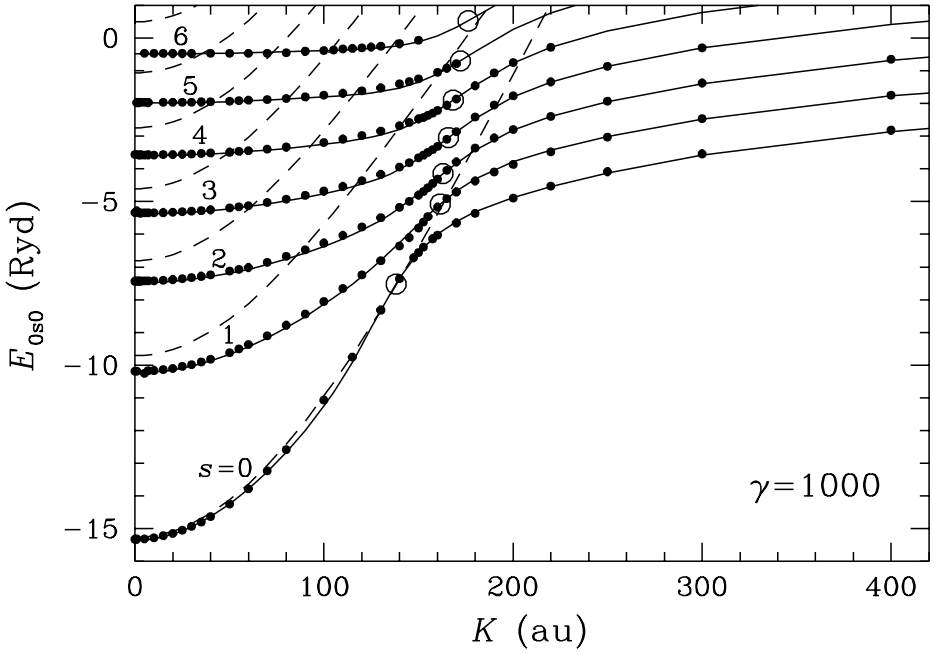

Figure 1. Energy spectrum of the hydrogen atom moving across strong magnetic fields. Numerical values (dots) are compared with the present analytical approximations (full lines) and with previously published[26] ones (dashed lines). Open circles mark the positions of K_c.

The function $E^{(2)}(K)$ that describes the longitudinal energy at large K is now

$$E^{(2)}_{0s\nu}(K) = \left\{ (2\ \mathrm{Ryd})^{-1} \left[r_*^2 + (2\nu+1) r_*^{3/2} + q_2 r_* \right]^{1/2} + 1/E^{(0)}_{0s\nu} \right\}^{-1}, \qquad (8)$$

with $q_2 = \nu^2 - 1$ for odd ν, and $q_2 = \nu^2 + 2^{\nu/2} \log_{10}(\gamma/300)$ for even ν (at $\gamma \geq 300$). The first and second terms in the square brackets ensure the correct asymptotic behavior.[15]

CONCLUDING REMARKS

The analytical approximations for binding energies presented in this contribution depend continuously on two arguments — magnetic field strength and transverse pseudomomentum. They are accurate, typically, within a few parts in 100–1000. The accuracy can be improved by almost an order of magnitude by optimizing the parameters m_{eff}, K_c, α, q_1, q_2 in equations (6)–(8) separately at each discrete value of γ. Tables of such optimized parameters have been obtained and will be published elsewhere, together with analytical approximations of geometrical sizes of various quantum-mechanical states of the moving atom and oscillator strengths of radiative transitions among them. The atomic sizes play important role in distribution of atoms over quantum states in a plasma and in their contribution to the plasma absorption coefficients. For example, a size of an atom may be used to evaluate effects of "unbounding" of electrons caused by random charge distribution in the plasma. For non-magnetized hydrogen plasma, an approximate treatment of these effects was revised recently;[27] for the strong magnetic fields analogous work is under way. Eventually, the analytical estimates of K-dependencies of the binding energies, atomic sizes, and transition rates help to generalize previously developed models of fully ionized atmospheres of magnetic neutron stars[28] to the more realistic case of partially ionized atmospheres.

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