Hydrogen atom in a magnetic field: quadrupole moment

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Abstract

Quadrupole moment of the hydrogen atom in a magnetic field $B = 0$–$4.414 \times 10^{13}$ G is calculated by two different methods. The first method is variational based on a single trial function. The second method deals with a solution of the Schrödinger equation in a form of a linear combination of the Landau orbitals.

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1 Introduction

Plenty of works were devoted to the hydrogen atom in a magnetic field (see, e.g., reviews [1–3]). This problem was among the first ones ever studied in quantum mechanics. To a great extent, a reason for such interest is due to its importance in various branches of fundamental physics: astrophysics, spectroscopy, solid state, and plasma physics. From the physical point of view, the first appearances of the influence of a magnetic field $B$ on the atom are (i) changes of binding energies, including the Zeeman level splitting which takes off the degeneracy, and (ii) a development of a non-vanishing quadrupole moment $Q_{ab} \propto B_a B_b$ as a consequence of a deformation of the spherical-symmetric atomic shape. In contrast to the former phenomenon, the latter one has not been thoroughly studied. Meanwhile, the appearance of the quadrupole moment leads to a drastic change in interaction of atoms. A standard van der Waals attraction originated from the interaction of induced dipoles is overtaken by the quadrupole-quadrupole interaction which is repulsive when atoms are situated along magnetic line (see [4,5]). In many applications (for instance, for construction of the equation of state), one needs to include the effects of atom-atom interactions. For example, a study of pressure ionization of a strongly magnetized hydrogen plasma is performed in [6] in a simple occupation probability model, which is based on a calculation of quantum-mechanical atomic sizes [7]. This model is fully adequate at sufficiently high temperatures $T$. However, in order to extend a domain of applicability to lower $T$, where neutral fraction is large, electrical multipole interactions of atoms should be taken into account. Therefore the quadrupole-quadrupole interaction can be significant at certain plasma parameters.

For various quantum-mechanical states of the H atom in a magnetic field, there have been accurate calculations of binding energies [8,9], oscillator strengths [10], and photoionization rates [11]. Moreover, binding energies [7,12,13], geometrical sizes and oscillator strengths [7,13], and photoionization cross sections [14] have been successfully calculated also for an atom moving in a strong magnetic field (equivalent to an atom in crossed magnetic and electric fields), which is an essentially three-dimensional system. Despite this progress, up to now the quadrupole moment was not basically studied with probably a single exception [15]. A goal of present Report is to carry out such a study for the ground state using (i) variational method and (ii) a method based on a solution of the Schrödinger equation by expansion in the Landau orbitals with coordinate-dependent coefficients. We explore the range of magnetic field strengths $B$ from 0 to the “relativistic” field $B_r \equiv m_e^2 c^3 / (\hbar \epsilon) = 4.414 \times 10^{13}$ G.

2 Asymptotic results

Hereafter, we will measure lengths in units of $a_0 \equiv h^2 / (m_e \epsilon^2) = 0.529177$ Å and energies in units of $\text{Ryd} \equiv 1/2 \epsilon^2 / a_0 = 13.6057$ eV. Assuming a constant uniform magnetic field directed along the $z$-axis, we take the vector potential
A in the symmetric (axial) gauge: \((A_x, A_y, A_z) = (B/2)(-y, x, 0)\). A natural parameter of the nonrelativistic theory is \(\gamma = B/B_0\), where \(B_0 \equiv m_e^2 c^3/(\hbar^3 c) = 2.3505 \times 10^9\) G. The field is called “strong” if \(\gamma \gtrsim 1\).

Since the magnetic quantum number equals zero for the ground state, the Hamiltonian has the form

\[
\mathcal{H} = -\Delta - \frac{2}{r} + \frac{\gamma^2}{4} \rho^2, \quad \rho^2 = x^2 + y^2.
\]

(1)

Because of the axial symmetry of the problem, the components \(Q_{\alpha\beta}\) of the quadrupole tensor obey the following relations (e.g., [16]):

\[
\begin{align*}
Q_{xy} &= Q_{yz} = Q_{zx} = 0, \\
Q_{xx} &= Q_{yy} = -\frac{1}{2}Q_{zz} = \langle z^2 \rangle - \langle x^2 \rangle.
\end{align*}
\]

(2)

In the weak-field limit, the usual perturbation theory gives [15]

\[-Q_{zz} \sim \frac{5}{2} \gamma^2 - \frac{615}{32} \gamma^4 + \ldots .
\]

(3)

In the opposite case of extremely strong field, \(\ln \gamma \gg 1\), when \(\langle x^2 \rangle \ll \langle z^2 \rangle\), the longitudinal motion can be separated, which gives rise to the one-dimensional model [17]. In the ground state, \(\langle z^2 \rangle\) is mainly determined by the exponential tail of the one-dimensional wavefunction: \(\langle z^2 \rangle \sim (2E)^{-1}\), where \(E\) is the binding energy. Using the method of Hasegawa and Howard [18] for evaluation of \(E\), we find

\[-Q_{zz} \sim \frac{1}{\ln \gamma} + \frac{2 \ln(\ln \gamma)}{(\ln \gamma)^3} + O\left(\frac{1}{(\ln \gamma)^3}\right)
\]

(4)

at \(\gamma \to \infty\).

3 Variational method

In order to construct an adequate variational trial function \(\Psi_0\), we follow a recipe formulated in [19–21]. Namely, the potential \(V_0 = (\Delta \Psi_0)/\Psi_0\) should reproduce the Coulomb singularity at the origin and the harmonic oscillator behavior at large distances. Furthermore, the trial function should have correct functional expansion in coordinates at small and large distances from the origin, as well as correct expansion in powers of \(B\). Since the ground state wavefunction has no nodal surfaces in the configuration space, we may write \(\Psi_0 = e^{-\phi}\), where \(\phi\) is a smooth real function of coordinates. Asymptotic behavior of this function has been calculated in [22, 15]:

\[
\phi = \begin{cases} 
\gamma \rho^2/4 + O(r) & (\rho \to \infty), \\
\gamma^2 (r^3 + \rho^2) + O(\gamma^4 r^3) & (r \to 0).
\end{cases}
\]

(5)
These expansions prompt to choose the following seven-parametric trial function:

\[
\Psi_0 = \exp \left\{ - \left[ a^2 \gamma^2 + (\alpha_1 \gamma^3 + \alpha_2 \gamma^2 + \alpha_3 \gamma + \alpha_4 \gamma^2) \right] \right\}
\]

(cf. [15, 21]), where \(a, \alpha_{1-4}, b_{1-2}\) are variational parameters. One can check that the effective potential \(V_0\) corresponding to this trial function reproduces correctly the potential in Eq. (1) at \(r \to 0\) (Coulomb regime) and at \(\rho \to \infty\) (Landau regime). Furthermore, Eq. (6) gives a correct functional form of the first corrections in powers \(B^2\) to the exponential phase of the ground-state wavefunction (see [22]) and, even more important, the functional form of the first correction to the Landau phase factor \(\propto B \rho^2\) at large distances (for a detailed discussion, see [15]). Thus, Eq. (6) takes into account the available information on the ground-state wavefunction of the Hamiltonian (1).

### 4 Expansion in Landau orbitals

The shape of the atom is close to a sphere at \(B \ll B_0\) and to a cylinder at \(B \gg B_0\). In the latter case, the expansion of the atomic wavefunction over the Landau functions is appropriate (e.g., [7, 8]).

If there were no Coulomb attraction, then the transverse part of the wavefunction could be described by a Landau function \(\Phi_{ns}(\rho, \varphi)\) (where \(\varphi\) is the polar angle in the \((xy)\)-plane) which satisfies the equation

\[
-\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \Phi_{ns}}{\partial \rho} \right) - \frac{1}{\rho^2} \frac{\partial^2 \Phi_{ns}}{\partial \varphi^2} + \frac{\gamma^2}{4} \Phi_{ns} = (2n + 1) \gamma.
\]

(e.g., [23]). Here, \(n\) is the Landau quantum number and \(s\) is the negative of the \(z\)-projection of the electron orbital momentum \((n \geq 0, s \geq -n)\). The Landau functions form a complete orthogonal functional basis on the \((xy)\)-plane.

When the atom does not move as a whole across the field, \(s\) is an exact quantum number. Thus a wavefunction \(\Psi\) can be presented as

\[
\Psi(\mathbf{r}) = \sum_n \Phi_{ns}(\rho, \phi) g_n(z).
\]

The sum in Eq. (8) if truncated at some \(n = N\) can be considered as a variational trial function. The one-dimensional functions \(g_n\) are to be found numerically. The minimum of the energy functional \(\langle \Psi | H | \Psi \rangle\) implies zero functional derivatives: \(\delta \langle \Psi | H | \Psi \rangle / \delta g_n(z) = 0\) \((\forall n)\). Taking into account Eq. (7), one arrives at a system of coupled differential equations for the set of \(g_n(z)\) and \(E\):

\[
\frac{d^2}{dz^2} g_n(z) + 2 \sum_{n'} V_{nn'}^{(s)}(z) g_{n'}(z) = (E + 2n \gamma) g_n(z),
\]
where

\[ V_{nn'}^{(s)}(z) = \int_0^\infty \rho \, d\rho \int_0^{2\pi} d\varphi \, \Phi_{ns}(\rho, \varphi) \frac{1}{r} \Phi_{n's}(\rho, \varphi). \]  

(10)

The effective potentials (10) can be reduced to a finite sum of one-dimensional integrals feasible for numerical calculation (e.g., [7]).

Using the relations

\[ \left( \begin{array}{c} x^2 \\ y^2 \end{array} \right) = r_+ r_- \pm \frac{1}{2} (r_+^2 + r_-^2), \]

(11)

\[ \sqrt{\gamma} r_+ \Phi_{ns} = \sqrt{n + s} \Phi_{n,s-1} - \sqrt{n + 1} \Phi_{n+1,s-1}, \]

\[ \sqrt{\gamma} r_- \Phi_{ns} = \sqrt{n + s + 1} \Phi_{n,s+1} - \sqrt{n} \Phi_{n-1,s+1}, \]

where \( r_\pm \equiv \rho e^{\pm i\varphi} \), one can calculate expectation values

\[ \langle z^2 \rangle = \sum_{n \geq 0} \int_{-\infty}^{\infty} z^2 |g_n(z)|^2 \, dz, \]

(12)

\[ \langle x^2 \rangle = \langle y^2 \rangle = \gamma \sum_{n \geq 0} \int_{-\infty}^{\infty} \left( (2n + s + 1) |g_n(z)|^2 - 2 \sqrt{(n + 1)(n + s + 1)} |g_n^*(z)g_{n+1}(z)| \right) \, dz. \]

(13)

and finally the quadrupole moment \( Q_{zz} \).

At \( \gamma \gg 1 \) the first term \( n = 0 \) dominates in the sum in Eq. (8). Hence Eq. (13) results in \( \langle x^2 \rangle = \langle y^2 \rangle \approx (s + 1)/\gamma \). It is worth to notice that neglecting all terms in Eq. (8) except one at \( n = 0 \) is equivalent to the adiabatic approximation used in early works (e.g., [1,18]).

5 Results and discussion

The results of our calculations of binding energy \( E \) and the quadrupole moment \( Q_{zz} \) are given in Table 1. When available we make comparison with the most accurate up-to-date results for the binding energy [9].

The variational approach of Sec. 3 based on a single seven-parametric function (6) gives very high relative accuracy in binding energy of the order of \( 10^{-7} \) at small magnetic fields which then falls to \( 10^{-2} \) at the largest studied magnetic fields. Basically, it corresponds to the same absolute accuracy \( 10^{-7} \) in the total energy for the whole explored range of magnetic fields. Two major parameters \( a, b_1 \) are changed as a function of magnetic field in very smooth and slow manner, from \( a \sim 1, b_1 \sim 0.9 \) for \( 10^9 \) G to \( a \sim 3, b_1 \sim 0.99 \) at \( 10^{13} \) G, respectively. Other parameters also vary smoothly and slow.

For the second method (Sec. 4), we retain \( n, n' = 0, 1, \ldots, 12 \) in the system of equations (9) and solve it for the ground state at \( \gamma \geq 1 \) using the algorithm described in Ref. [7]. Then we calculate \( Q_{zz} \) from Eq. (2) using Eqs. (12), (13).

From Table 1, we see that the method of expansion in the Landau orbitals turns out to be more accurate at \( \gamma \gtrsim 10 \), whereas the variational method of
Sec. 3 is superior at lower field strengths. This is confirmed by comparison with the results of Ref. [9]. Both methods give very close results for the quadrupole moment.

The data in Table 1 can be approximated by the expression

\[
-Q_{zz} \approx \frac{\xi \gamma^{7/4}}{0.3488 + (1 + \xi^3) \gamma^{7/4}}, \tag{14}
\]

where \( \xi = 4 \ln(1 + 0.218 \gamma^{1/4}) \).

This approximation reproduces the exact asymptotic behavior: \(-Q_{zz} \sim \ln(\gamma)^{-2}\) at \( \gamma \to \infty \) and \( -Q_{zz} \sim \frac{4}{3} \gamma^2 \) at \( \gamma \to 0 \). Its deviation from the results in the Table does not exceed a few percent in the whole range of studied magnetic fields.

Figure 1 shows \(|Q_{zz}|\) as a function of \( \gamma \). Numerical results obtained as described in Sec. 3 (shown by dots) and Sec. 4 (solid line) are compared with the perturbation theory of order \( B^2 \) and \( B^4 \) (lines marked “1” and “2”, respectively) and with the fit (14) (dashed line). The quadrupole moment grows smoothly with magnetic field increase reaching maximum at \( \gamma \approx 3 \) and then decreases. We note, however, that the van der Waals constant decreases at \( \gamma \to \infty \) as \( (\ln \gamma)^{-4} \) i.e., at the same rate as \( Q_{zz}^2 \). This means that the distance \( R \) where the van der Waals potential \( \propto R^{-6} \) becomes comparable with the quadrupole-quadrupole potential \( \sim Q^2/R^5 \) tends to a finite value at \( \gamma \to \infty \). Our results may have important impact on modeling of relatively cool neutron star atmospheres, whose spectra are being measured with the X-ray telescopes onboard recently launched *Chandra* and *XMM-Newton* space observatories.

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### References

Figure 1: Absolute value of the quadrupole moment $Q_{zz}$ as function of $\gamma = B/(2.35 \times 10^9 \text{ G})$: numerical results are compared with perturbation theory (3) and analytic fit (14).

Table 1: Binding energy $E$ and absolute value of the quadrupole moment $Q_{zz}$ at different magnetic fields $B$ calculated (a) by the variational method and (b) by expansion in the Landau basis. Rounded-off data from Ref. [9] are given for comparison.

<table>
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<th>$B$</th>
<th>$E$ (Ryd)</th>
<th>$Q_{zz}$ (a.u.)</th>
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<tr>
<td></td>
<td>(a)</td>
<td>(b)</td>
</tr>
<tr>
<td>$0.1 B_0$</td>
<td>1.09505274</td>
<td>–</td>
</tr>
<tr>
<td>$10^9$ G</td>
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<td>–</td>
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<td>$B_0$</td>
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<td>3.490</td>
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