Hydrogen atom in a magnetic field: The quadrupole moment

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The quadrupole moment of a hydrogen atom in a magnetic field B for field strengths from 0 to 4.414×10^{13} G is calculated by two different methods. The first method is variational, and based on a single trial function. The second method deals with a solution of the Schrödinger equation in the form of a linear combination of Landau orbitals.

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I. INTRODUCTION

Plenty of works has been devoted study of a hydrogen atom in a magnetic field (see, e.g., Refs. [1–3]) and this problem was among the first ever studied in quantum mechanics. To a great extent, the reason for such interest is due to its importance in various branches of fundamental physics: astrophysics, spectroscopy, solid state, and plasma physics. From a physical point of view, the first appearances of the influence of a magnetic field B on the atom are (i) changes in binding energies, including the Zeeman level splitting which removes a degeneracy; and (ii) the development of a nonvanishing quadrupole moment $Q_{ab}\propto B_aB_b$ as a consequence of the deformation of the spherical-symmetrical atomic shape. In contrast to the former phenomenon, the latter has not been thoroughly studied. Meanwhile, the appearance of a quadrupole moment leads to a drastic change in the interaction of the atoms. A standard van der Waals attraction which originates in the interaction of induced dipoles is overtaken by quadrupole-quadrupole interaction (which is repulsive when atoms are situated along magnetic line — see Refs. [4,5]). In many applications (for instance, for construction of an 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 was performed in Ref. [6] with a simple occupation probability model, which was 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 the domain of applicability to lower T, where the neutral fraction is large, electrical multipole interactions of atoms should be taken into account. Therefore, 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], electric quadrupole transition probabilities [14], and photoionization cross sections [15] have also been successfully calculated 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 studied basically with perhaps a single exception [16]. A goal of the present Brief Report is to carry out such a study for the ground state using (i) a variational method, and (ii) a method based on a solution of the Schrödinger equation by expansion in Landau orbitals with coordinate-dependent coefficients. We explore a range of magnetic field strengths B from 0 to the ''relativistic'' field $B_r\equiv m_e^2c^3/(\hbar e)=4.414\times10^{13}$ G.

II. ASYMPTOTIC RESULTS

Hereafter, we will measure lengths in units of $a_0\equiv\hbar^2/(m_ee^2)=0.529\,177$ Å and energies in units of Ry $\equiv\frac{1}{2}e^2/a_0=13.6057$ eV. Assuming a constant uniform magnetic field directed along the z axis, we take the vector potential $\mathbf{A}$ 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 $B_0\equiv m_e^2e^3/(\hbar^3c)=2.3505\times10^9$ G. The field is called ''strong'' if $\gamma\gtrsim1$.

Since the magnetic quantum number is equal to zero for the ground state, the Hamiltonian has the form

$$\mathcal{H}=-\Delta-\frac{2}{r}+\frac{\gamma^2}{4}\rho^2,\quad \rho^2=x^2+y^2. \tag{1}$$

Because of the axial symmetry of the problem, the components $Q_{\alpha\beta}$ of the quadrupole tensor obey the following relations (e.g., Ref. [17]):

$$Q_{xy}=Q_{yz}=Q_{zx}=0,$$

$$Q_{xx}=Q_{yy}=-\frac{1}{2}Q_{zz}=\langle z^2\rangle-\langle x^2\rangle. \tag{2}$$

In the weak-field limit, the usual perturbation theory gives [16]

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$$-Q_{zz}=\frac{5}{2}\gamma^2-\frac{615}{32}\gamma^4+\cdots. \tag{3}$$

In the opposite case of an ultrastrong field, $\ln\gamma\gg1$, when $\langle x^2\rangle\ll\langle z^2\rangle$, the longitudinal motion can be separated, which gives rise to the one-dimensional model [18]. In the ground state, $\langle z^2\rangle$ is mainly determined by the exponential tail of the one-dimensional wave function, $\langle z^2\rangle\sim(2E)^{-1}$, where E is the binding energy. Using the method of Hasegawa and Howard [19] for an evaluation of E, we find

$$-Q_{zz}\sim\frac{1}{(\ln\gamma)^2}+\frac{2\ln(\ln\gamma)}{(\ln\gamma)^3}+O\left(\frac{1}{(\ln\gamma)^3}\right) \tag{4}$$

at $\gamma\to\infty$.

III. VARIATIONAL METHOD

In order to construct an adequate variational trial function Ψ_0, we follow a recipe formulated in Refs. [20–22]. That is, the potential $V_0=(\Delta\Psi_0)/\Psi_0$ should reproduce the Coulomb singularity at the origin, and harmonic-oscillator behavior at large distances. Furthermore, the trial function should have a correct functional expansion in coordinates at small and large distances from the origin, as well as a correct expansion in powers of B. Since the ground-state wave function has no nodal surfaces in configuration space, we may write $\Psi_0=e^{-\phi}$, where ϕ is a smooth real function of coordinates. The asymptotic behavior of this function was calculated in Refs. [23,16]:

$$\phi=\gamma\rho^2/4+O(r)\quad(\rho\to\infty), \tag{5}$$

$$\phi=r+\gamma^2(Ar^3+Br\rho^2+Cr^2+D\rho^2)+O(\gamma^4r^5)\quad(r\to0), \tag{6}$$

where A,B,C, and D are known parameters. These expansions prompt to choose the seven-parametric trial function

$$\Psi_0=\exp\{-[a^2r^2+(\alpha_1r^3+\alpha_2\rho^2r+\alpha_3\rho^3+\alpha_4\rho r^2)\gamma+(b_1\rho^4+\ b_2\rho^2r^2)\gamma^2/16]^{1/2}\}, \tag{7}$$

(cf. Refs. [16,22]), where a,α_{1-4}, and b_{1-2} are variational parameters. One can check that the effective potential V_0 corresponding to this trial function correctly reproduces the potential in Eq. (1) at $r\to0$ (Coulomb regime) and at $\rho\to\infty$ (Landau regime). Furthermore, Eq. (7) gives a correct functional form of the first corrections in powers B^2 to the exponential phase of the ground-state wave function (see Ref. [23]) and, even more importantly, the functional form of the first correction to the Landau phase factor $\propto B\rho^2$ at large distances (for a detailed discussion, see Ref. [16]). Thus Eq. (7) takes into account the available information on the ground-state wave function of Hamiltonian (1).

IV. 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 wave function over the Landau functions is appropriate (e.g., Refs. [7,8]).

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

$$-\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Phi_{ns}}{\partial\rho}\right)-\frac{1}{\rho^2}\frac{\partial^2\Phi_{ns}}{\partial\varphi^2}+\frac{\gamma^2}{4}\Phi_{ns}=(2n+1)\gamma. \tag{8}$$

(e.g., Ref. [24]). Here n is the Landau quantum number and s is the negative of the z projection of the electron orbital momentum ($n\geqslant0,\ s\geqslant-n$). 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 wave function Ψ can be presented as

$$\Psi(\mathbf{r})=\sum_n\ \Phi_{ns}(\rho,\phi)g_n(z). \tag{9}$$

The sum in Eq. (9), 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 $\langle\Psi|\mathcal{H}|\Psi\rangle$ implies zero functional derivatives: $\delta\langle\Psi|\mathcal{H}|\Psi\rangle/\delta g_n(z)=0\ (\forall n)$. Taking into account Eq. (8), one arrives at a system of coupled differential equations for the set of $g_n(z)$ and E,

$$\frac{d^2}{dz^2}g_n(z)+2\sum_{n'}\ V^{(s)}_{nn'}(z)g_{n'}(z)=(E+2n\gamma)g_n(z), \tag{10}$$

where

$$V^{(s)}_{nn'}(z)=\int_0^\infty\rho d\rho\int_0^{2\pi}\mathrm{d}\varphi\Phi^*_{ns}(\rho,\varphi)\frac{1}{r}\Phi_{n's}(\rho,\varphi). \tag{11}$$

The effective potentials [Eq. (11)] can be reduced to a finite sum of one-dimensional integrals feasible for numerical calculation [7].

Using the relations

$$\begin{pmatrix}x^2\\y^2\end{pmatrix}=r_+r_-\pm\frac{1}{2}(r_+^2+r_-^2), \tag{12}$$

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

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

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

$$\langle z^2\rangle=\sum_{n\geqslant0}\int_{-\infty}^{\infty}z^2|g_n(z)|^2dz, \tag{13}$$

TABLE I. 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.

B	E (Ry)			$-Q_{zz}$(a.u.)	
	(a)	(b)	Ref. [9]	(a)	(b)
$0.1B_0$	1.095 05274	–	1.095 05296	0.0235	–
10^9 G	1.346 292	–		0.2185	–
B_0	1.662 322	1.63	1.662 338	0.4155	0.38
10^{10} G	2.614 73	2.61		0.5085	0.48
$10\,B_0$	3.4948	3.490	3.495 6	0.4370	0.447
10^{11} G	5.713	5.717		0.2806	0.290
$100\,B_0$	7.5642	7.579	7.579 6	0.2071	0.217
10^{12} G	11.87	11.924		0.1228	0.1308
$1000\,B_0$	15.23	15.325	15.324 9	0.0915	0.0981
10^{13} G	22.5	22.77		0.0576	0.0620
B_r	32.5	32.92		0.0380	0.0406

$$\langle x^2\rangle=\langle y^2\rangle = \gamma\sum_{n\geqslant 0}\int_{-\infty}^{\infty}[(2n+s+1)|g_n(z)|^2 - 2\sqrt{(n+1)(n+s+1)}|g_n^*(z)g_{n+1}(z)|]dz. \quad (14)$$

and finally the quadrupole moment Q_{zz}.

At $\gamma\gg 1$ the first term $n=0$ dominates in the sum in Eq. (9). Hence Eq. (14) results in $\langle x^2\rangle=\langle y^2\rangle\approx(s+1)/\gamma$. It is worthwhile to note that neglecting all terms in Eq. (9) except the one at $n=0$ is equivalent to the adiabatic approximation used in early works (e.g., Refs. [1,19]).

V. RESULTS AND DISCUSSION

The results of our calculations of the binding energy E and the quadrupole moment Q_{zz} are presented in Table I. When available, we compare the binding energy with the most accurate up-to-date results [9].

The variational approach of Sec. III, based on a *single* seven-parametric function [Eq. (7)], gives a very high relative accuracy in the binding energy on the order of 10^{-7} at small magnetic fields, which then falls to 10^{-2} at the largest studied magnetic fields. Basically, this corresponds to the same absolute accuracy (on the order of 10^{-7}) in the *total* energy for the whole explored range of magnetic fields. Two major parameters a and b_1 are changed as a function of magnetic field in a 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 slowly.

For the second method (Sec. IV), we retain $n,n'=0,1,\ldots,12$ in the system of equations (10) and solve it for the ground state at $\gamma\geqslant 1$ using the algorithm described in Ref. [7]. Then we calculate Q_{zz} from Eq. (2) using Eqs. (13) and (14).

In Table I we see that for the binding energy the method of expansion in the Landau orbitals turns out to be more accurate at $\gamma\gtrsim 10$, whereas the variational method of Sec. III is superior at lower field strengths. This is confirmed by a comparison with the results of Ref. [9]. We emphasize that our methods give very close results for the quadrupole moment. This agrees with the qualitative behavior found in [16].

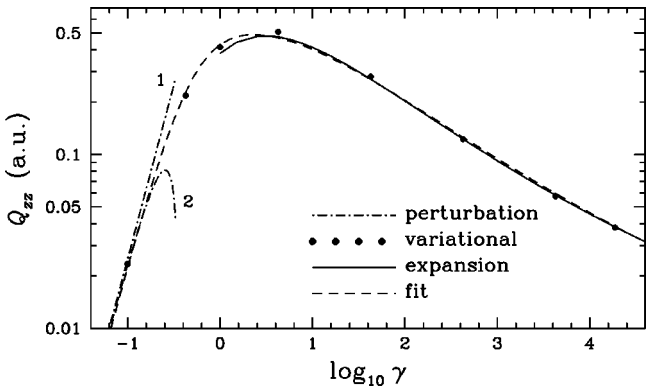

FIG. 1. Absolute value of the quadrupole moment Q_{zz} as a function of $\gamma=B/(2.35\times 10^9$ G), calculated by the variational method (Sec. III) and the Landau orbital expansion approach (Sec. IV): numerical results are compared with perturbation theory [Eq. (3)] [curve 1 corresponds to the first term in Eq. (3), and curve 2 to two terms] and the analytic fit [Eq. (15)]. At $\gamma\to 0$ the quadrupole moment Q_{zz} tends to zero.

The data in Table I can be approximated by the expression

$$-Q_{zz}\approx\frac{\xi\gamma^{7/4}}{0.3392+(1+\xi^3)\gamma^{7/4}}, \quad (15)$$

where

$$\xi=4\ln(1+0.212\gamma^{1/4}).$$

This approximation reproduces the exact asymptotic behavior: $-Q_{zz}\sim(\ln\gamma)^{-2}$ at $\gamma\to\infty$ and $-Q_{zz}\sim\frac{5}{2}\gamma^2$ at $\gamma\to 0$. Its deviation from the results in Table I does not exceed a few percent in the whole range of studied magnetic fields.

Figure 1 shows $|Q_{zz}|$ as a function of γ. Numerical results obtained as described in Secs. III (shown by dots) and IV (solid line) are compared with perturbation theories of order B^2 and B^4 (lines marked '1' and '2', respectively) and with the fit [Eq. (15)] (dashed line). The quadrupole moment grows smoothly with magnetic field increase, reaching the maximum at $\gamma\approx 3$ and then decreases. For the strongly elongated atom at $\gamma\gg 1$, the van der Waals constant can be roughly estimated as $W\sim E\langle z^2\rangle^3\propto(\ln\gamma)^{-4}$. Thus W decreases at $\gamma\to\infty$ at the same rate as Q_{zz}^2. This means that the distance R, where the van der Waals potential $\sim W/R^6$ becomes comparable with the quadrupole-quadrupole interaction potential $\sim Q^2/R^5$, tends to a finite value at $\gamma\to\infty$. Our results may have an important impact on the modeling of relatively cool neutron star atmospheres, whose spectra are being measured with the x-ray telescopes onboard the recently launched *Chandra* and *XMM-Newton* space observatories (e.g., Refs. [25,26]).

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