Quantization rules and instabilities of highly excited hydrogen atom in a strong magnetic field

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The quantization rules and instability regions are found for highly excited, concentrated states of atomic hydrogen in a strong magnetic field. The corresponding dipole matrix elements for transitions from the ground state oscillate as a function of the magnetic field; the oscillations have a high peak and a minimum near the boundaries of the regions.

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The study of highly excited atoms in a strong magnetic field, such that the magnitude of the field is comparable to or greater than the distance between levels (see Refs. 1–4 and the references therein), has recently been of special interest. For weak (in the classical sense) fields, it is possible to use classical perturbation theory.[5,6] However, as the magnetic field increases, this theory becomes inapplicable. The adiabatic approximation, on the contrary, imposes an extremely low lower bound on the magnetic field and ignores the important three-dimensional properties of the motion of the electron in superposed Coulomb and oscillating fields.[4]

We shall examine the highly excited states of an electron concentrated near the z axis, which coincides with the direction of the magnetic field B. We shall expand the potential $V = -1/r + \gamma^2\rho^2/8$ ($\gamma = B/B_0$, $B_0 = 2.35\times 10^5$ T) for z much greater than the characteristic transverse dimension ρ_0 of the bound state up to terms quadratic in ρ ($r=\sqrt{z^2+\rho^2}$). After separating out the azimuthal factor $\exp(im\phi)$ and introducing the time variable, the Schrödinger equation in this region,

$$\tau = \int^z \frac{dz}{p},\; p = \sqrt{\frac{2}{z} - \epsilon^2},\; \epsilon^2 = \gamma m - 2E,\; m = 0, \pm 1, \pm 2, \dots,$$

is transformed into a nonstationary Schrödinger equation for a harmonic oscillator with a variable frequency, admitting separation of variables.[7] Near the center of the hydrogen atom, at distances less than or of the order of ρ_0, we shall ignore the magnetic field and assume that the potential is purely Coulombic. The magnetic field in this case must be limited from above by inequality (3). Then we join the solutions obtained at $z\sim\rho_0$ to a linear combination of Coulomb solutions and we find the eigenfunctions of the problem (which are expressed in terms of a sum of products of Jacobi and Laguerre polynomials of complex arguments and which are not presented here due to their cumbersome nature). This leads, in particular, to the quantization rule[6]

$$\int_0^{\epsilon^{-2}} p\,dz = \pi n + \frac{\mu}{2}(2k + |m| + 1), \quad n >> 2k + |m| + 1, \quad k \geqslant 0; \quad k, n - \text{integers} \tag{1}$$

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where μ is the characteristic index of the differential equation linearized with respect to ρ for the classical trajectories $\rho(z)$, next to the z axis:

$$u^2(1-u)^2(\rho\sqrt{\rho})_{uu} + \left[\frac{3}{16} + \kappa u^3(1-u)\right](\rho\sqrt{\rho}) = 0, \quad \kappa = \frac{\gamma^2}{\epsilon^6}, \quad u = \frac{\epsilon^2 z}{2}. \tag{2}$$

If $\gamma = 0$, then $\mu = 0$ and we obtain from (1) the Coulomb energy spectrum. In what follows, we shall assume that $\gamma n^3 \gg 1$. Thus, the approximation examined in this paper is valid for

$$\left(\frac{n}{2k+|m|+1}\right)^{3/2} \gg \gamma n^3 \gg 1, \tag{3}$$

as well as outside some neighborhood of the resonance points (see below).

In the region $ku^3 \gg 1$, we solve Eq. (2) using the WKB method and then we join these solutions with the solutions (2) near the center, where the magnetic field can be ignored. As a result, (1) takes the form

$$\frac{\pi}{\epsilon} = \pi n + (2k+|m|+1)\,\mathrm{arctg}\sqrt{\mathrm{tg}\left(\frac{\pi\sqrt{\kappa}}{2} + \frac{\pi}{3}\right)\mathrm{tg}\left(\frac{\pi\sqrt{\kappa}}{2} - \frac{\pi}{3}\right)}. \tag{4}$$

The phase $\pi/3$ appears in (4) due to the Coulomb core of the potential. It is evident from (4) that the characteristic index μ is real in the regions

$$\gamma_{nq}^- < \gamma < \gamma_{nq}^+, \qquad \gamma_{nq}^{\pm} = \epsilon^3\left(\frac{1}{2} \pm \frac{1}{6} + q\right) \qquad n, q \gg 1 - \text{integers}, \tag{5}$$

and outside these regions the concentrated motion near the z axis becomes unstable in phase space. The boundaries of the regions of stability correspond to the classical resonances and, for $\mu = 0$, to the energy spectrum

$$E_{nmq}^{\pm} = -\frac{1}{2n^2} + \frac{m}{2n^3}\left(\frac{1}{2} \pm \frac{1}{6} + q\right), \tag{6}$$

which coincides for $m = 0$ with the Coulomb spectrum. Let us set, for example, $n = 100$, $q = 10, 11, 12, \ldots$. Thus, the magnetic field, which corresponds to $\gamma_{100,q'}^{+}$, assumes the values 2.51, 2.74, 2.98,... T.

For γ close to $\gamma_{nq}^{\pm}$, the wave functions spread out as a function of ρ and the method used by us is valid only for $\rho_0 \ll n^2$ or for

$$|\gamma - \gamma_{nq}^{\pm}| \gg \frac{(2k+|m|+1)^2}{\gamma^2 n^{11}}. \tag{7}$$

On the other hand, the values of the magnetic field $\gamma = \gamma_{nq}^{\pm}$ correspond to $\mu = 0$, i.e., to pseudocrossing points, which, according to (4), are simply a crossing. The quantization rule (4), like the quasiclassical rule, is valid outside neighborhoods of pseudocrossing points, determined by the estimate $\mu \gg 1/n$ or

$$|\gamma - \gamma_{nq}^{\pm}|^{1/2} \gg n^{-5/2}. \tag{8}$$

This inequality for $k, m \sim 1$ is stronger than (7).

The expression obtained for the eigenfunctions of the electron leads to simple equations for the dipole matrix elements. For a transition from the ground state ψ_0 to a highly excited state with $m = 0$, we have

$$|<\psi_0|z|\psi_{0nk}>|^2 = \frac{2^{11}3^{2/3}\pi}{e^4\Gamma^2\left(\frac{1}{6}\right)}\frac{\gamma^{1/3}}{n^3}\beta^{1/2}, \quad \beta = \frac{\sin\left(\pi\sqrt{\kappa} - \frac{2\pi}{3}\right)}{\sin\left(\pi\sqrt{\kappa} + \frac{2\pi}{3}\right)}, \tag{9}$$

and for the analogous transition to the state with $m = \pm 1$, we have

$$|<\psi_0|x|\psi_{\pm 1, nk}>|^2 = \frac{2^{13}3^{4/3}\pi^2(k+1)}{e^4\Gamma^4\left(\frac{1}{6}\right)}\frac{\gamma^{2/3}}{n^3}\beta. \tag{10}$$

The remaining transitions from the ground state are forbidden according to the selection rules. The oscillatory, as a function of the magnetic field (and, with fixed γ, as a function of n), behavior of the oscillator strengths is evident from (9) and (10). The values of the oscillator strengths for $\gamma = 2\times 10^{-5}$ and $n = 23,...50$ (and $\gamma n^3 < 2.5$) were obtained numerically in Ref. 1. The dependence of the oscillator strengths on n, according to Ref. 1, turns out to be monotonic for $\gamma n^3 < 1$ and irregularities appear in the tail of the spectrum studied, after strong mixing for $\gamma n^3 \sim 1$. The results (9) and (10) correspond, as noted, to the case $\gamma n^3 \gg 1$ and describe the behavior of the oscillator strengths in the regions of stability. At the boundary of the region with $\gamma = \gamma_{nq}^-$, expressions (9) and (10) have a singularity, resulting from the classical resonance. The relative magnitude of the increase in intensity is determined by the factor $\beta^{1/2}$ for $m = 0$ and by the factor β for $m = \pm 1$. Near the resonance, we have

$$\beta \approx 0{,}28(\gamma - \gamma_{nq}^-)^{-1}n^{-3}. \tag{11}$$

Equation (11) is valid under conditions (7) and (8). The maximum value of β can be estimated by setting $\mu \gtrsim 1/n$, from which we obtain $\beta \lesssim n^2$.

In conclusion, we note that if the phases $\pi/3$ are dropped in the quantization rule (4), then it goes over into the result obtained with the adiabatic approximation, since in this case $\arctan(...) = \pi\gamma\epsilon^{-3}/2$. These phases can be dropped if the inequality opposite to the first one in (3) is satisfied, i.e., if the magnetic field is very strong.

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