

Highly excited hydrogen-atom states located in an external field near the symmetry axis of the field

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Quantization rules are obtained and bands of stability loss in a strong magnetic field as well as in parallel electric and magnetic fields are observed for highly excited hydrogen states concentrated near the symmetry axis of the external field. The band boundaries are identical with the classical resonances at which a classical trajectory lying on the symmetry axis loses stability. The calculation is based on matching of the Schrödinger-equation solutions that are valid near the center of the atom with those valid at a distance from the center and concentrated near the field symmetry axis. The elements of the dipole transitions from the ground state to highly excited states are calculated. In the case of a weak magnetic field the oscillator strengths obtained agree well with the numerical calculations of Clark and Taylor [J. Phys. **13B**, L737 (1980)]. For a strong magnetic field as well as for sufficiently weak parallel electric and magnetic fields the oscillator strengths show a spike near one stability-band boundary and a dip near the other.

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The properties of highly excited atoms in constant electric and magnetic fields that produce a level shift larger than or of the order of the distance between the levels in the absence of a field have been recently investigated in many theoretical and experimental studies (see the reviews^{1,2} as well as Refs. 3–10). The investigation of such systems even in the one-electron approximation (except for the hydrogen atom in a constant electric field) reduces to a solution of a Schrödinger equation with nonseparable variables. A numerical solution of the problem can be obtained with good accuracy for low-lying levels. With increasing quantum numbers, however, the known numerical methods for calculating the terms become unreliable. The use of quasiclassical perturbation theory, which is natural for highly excited states and for a sufficiently weak external field, likewise encounters a number of difficulties, such as the problem of small denominators, the presence of an irregular spectrum, and others. The adiabatic approximation, conversely, imposes an exceedingly stringent lower bound on the magnetic field and does not take into account the essential three-dimensional singularities of electron motion in a superposition of Coulomb and oscillator fields.⁴

This paper considers in a quasiclassical approximation highly excited states of the hydrogen atom (hydrogenlike ion) in a constant magnetic field. The states are concentrated along the symmetry axis of the field. This concentration can arise, for example, in a sufficiently strong magnetic field, or can be preserved when concentrated states of the atoms are perturbed. We consider states with a large longitudinal and a small transverse momentum. We obtain for such states expression, quantization rules, as well as the values of the dipole matrix elements.

In Secs. 1 and 2 we expound the method of solving the Schrödinger equation for the state considered and derive thereby quantization rules and expressions for the wave functions.

The equations derived are used in Sec. 3 to calculate the

levels of a hydrogen atom in a magnetic field. A term quadratic in the field is obtained in the case of a weak field. The quantization rule for a strong magnetic field can be reduced to the form (29). It is shown that when the field is varied the stability regions of the considered states form bands whose boundaries coincide with the classical resonances. As a boundary is approached, the wave functions considered spread out in opposite directions. The physical cause of the existence of such bands is that when the magnetic field is varied the trajectory located on the symmetry of the axis loses and regains stability periodically.

It is shown in Sec. 4 that the phenomenon caused by the loss of the stability of the states localized near the symmetry axis of the potential takes place also in sufficiently weak parallel electric and magnetic fields. An expression for the energy levels in the stability bands is obtained for this case. Also considered here is the case of strong parallel magnetic and electric fields.

Section 5 is devoted to a calculation of the oscillator strengths for transitions from the ground state into the considered highly excited states. In the case of a weak electric field the equations obtained coincide with the known ones.¹¹ Good agreement with the numerical results of Ref. 3 is obtained also for a weak magnetic field. The oscillator strengths are calculated for a strong magnetic field. It is shown that the radiation intensity has a spike near one of the stability-band boundaries, and a dip near the other. Expressions are also obtained for oscillator strengths in weak parallel electric and magnetic field. In this case, too, the radiation intensity has a spike or is damped near a stability-band boundary.

1. DESCRIPTION OF METHOD

Let the wave function of an electron be concentrated in the vicinity of the symmetry axis z of the potential. For the highly excited states considered in this paper, with large longitudinal quantum numbers n (which will be determined be-

low), the solution of the Schrödinger equation

$${}^{1/2}\Delta\Psi + (E - V)\Psi = 0, \quad V(z, \rho) = -\alpha(z^2 + \rho^2)^{-1/2} + W(z, \rho) \quad (1)$$

can be obtained in the following manner. We divide the region of electron motion into two. The first is localized near the atom center, and here we neglect the external field $W(x, \rho)$, i.e., a pure Coulomb potential is assumed. The second is localized near the z axis. In this region we assume that $\rho \ll z$ and expand the potential, accurate to terms quadratic in ρ :

$$V(z, \rho) = V^0(z) + {}^{1/2}\rho^2 V_{\rho\rho}^0(z). \quad (2)$$

The solution is sought by the parabolic-equation method.¹² The solutions indicated are then joined and it is required that the obtained wave function decrease exponentially at large $|z|$ and ρ . As a result we obtain the eigenfunctions and the quantization rules.

We consider first classical motion near the symmetry axis of the potential. The equation for the classical trajectories $\rho(z)$ takes in the approximation linear in ρ the form

$$\rho_{zz} + (p_z/p)\rho_z + (V_{\rho\rho}^0/p^2)\rho = 0, \quad p(z) = [2(E - V^0(z))]^{1/2}. \quad (3)$$

This equation is derived in Appendix 1. It is valid if $\rho \ll z$ and also if $\rho_z \ll 1$, i.e., the corresponding classical trajectories must be close in phase space to the trajectory lying on the z axis. We shall find it more convenient to rewrite this equation in reduced form

$$y_{zz} + (p_z^2/4p^2 - p_{zz}/2p + V_{\rho\rho}^0/p^2)y = 0, \quad y(z) = \rho(z)(p(z))^{1/2}. \quad (4)$$

In the first region, where a Coulomb potential is assumed, Eq. (4) can be solved exactly. The corresponding solutions are

$$y_1^0(z) = zp^{1/2}, \quad y_2^0(z) = (z/\alpha)p^{3/2}, \quad w(y_1^0, y_2^0) = 1 \quad (5)$$

(w is the Wronskian). It is easily seen that these solutions define classical trajectories $\rho(z)$ for a Coulomb field, with a small orbital momentum.

Equation (4) can also be solved near the momentum turning point $z_1(p/z_1) = 0$. In fact, as $z \rightarrow z_1$ the first two terms in the parentheses of (4) become much larger than the third. Neglecting the latter, we obtain the following solutions:

$$y_1^1(z) = p^{1/2}, \quad y_2^1(z) = p^{1/2} \int_{z_1}^z \frac{dz}{p}, \quad w(y_1^1, y_2^1) = 1. \quad (6)$$

These solutions correspond to classical trajectories with small transverse energy, for a potential that depends only on z .

Let y_1 and y_2 be solutions of (4) that go over at small z respectively to the solutions (5). The functions y_1 and y_2 then go over in the vicinity of the turning point z_1 into linear combinations of the solutions (6). We define now the constant matrix \mathbf{T} by means of equation

$$y_{z \rightarrow z_1} \approx \mathbf{T}y^1, \quad y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad y^1 = \begin{pmatrix} y_1^1 \\ y_2^1 \end{pmatrix}, \quad \mathbf{T} = \|t_{ij}\|. \quad (7)$$

This matrix transforms the solutions of Eqs. (3) and (4), which are valid in the Coulomb region, into solutions near

the turning point z_1 . The quantization rules obtained below, as well as the values of the dipole matrix elements of the transitions into the considered highly excited states, are uniquely defined in terms of the elements t_{ij} of this matrix.

The classical-trajectory equation (3) does not hold in the immediate vicinity of the center and of the point z_1 . Joining together the solutions in these regions, we can, knowing the matrix \mathbf{T} , find the boundaries of the stability regions of the states in question; these boundaries coincide with the classical resonances (see Appendix 1).

2. QUANTIZATION RULE AND EIGENFUNCTIONS

To determine the eigenfunctions, we find the solutions of the Schrödinger equation in the regions indicated above, and then join them in the region where they overlap.

In the first region, where a pure Coulomb potential is assumed, particular solutions are obtained in the form of products of Laguerre polynomials and confluent hypergeometric functions:

$$\Phi_{m_k}^{\text{Coul}}(\mathbf{r}) = e^{im\varphi}(\xi\eta)^{|m|/2} \exp\left[-\frac{\kappa}{2}(\xi+\eta)\right] L_k^{|m|}(\kappa\eta) \times F(k+|m|+1-\alpha/\kappa, |m|+1, \kappa\xi), \quad \kappa^2 = -2E, \quad (8)$$

where ξ and η are parabolic coordinates. The wave functions (8) tend to zero both at large ρ and as $z \rightarrow -\infty$. Therefore linear combinations of such functions satisfy the boundary conditions for the eigenstates as $\rho \rightarrow \infty$ and as $z \rightarrow -\infty$.

In the second region, where it is assumed that $z \gg \rho$, and also that $z \gg n(2k + |m| + 1)/\alpha$, the solution can be obtained by the parabolic-equation method^{11,13}:

$$\Psi_{m_k}(\mathbf{r}) = \frac{e^{im\varphi}}{\sigma} \left(\frac{\rho p^{1/2}}{\sigma}\right)^{|m|} L_k^{|m|}\left(\frac{\rho^2 p}{\sigma^2}\right) \times \exp\left[i \int_0^z \left(p - \frac{2k+|m|+1}{\sigma^2}\right) dz + \frac{i\rho^2 p}{2} \left(\frac{\sigma_z}{\sigma} + \frac{i}{\sigma^2} - \frac{p_z}{2p}\right)\right]; \quad k, |m| = 0, 1, 2, \dots \quad (9)$$

Here $\sigma^2(z)$ is a quadratic form made up of the solutions, indicated in the preceding section, of Eq. (4):

$$\sigma^2(z) = \sum_{j,i=1}^2 a_{ji} y_j(z) y_i(z) = (\mathbf{A}y, y), \quad \det \mathbf{A} = 1, \quad (10)$$

\mathbf{A} is a symmetric matrix of the free parameters, with a unity determinant. The solution (9) was obtained in a quasiclassical approximation with respect to z . Just as Eq. (3), it is valid if the transverse-momentum component is much less than the longitudinal one, and takes into account their ratio to first order.

The plan of the subsequent calculations is the following. We join together linear combinations of the solutions (8) and (9), and then stipulate an exponential decrease of the obtained solution as $z \rightarrow +\infty$. As a result we obtain the eigenfunction of the problem considered.

We use the asymptotic form of (8) as $\alpha/\kappa \rightarrow \infty$ (highly excited states) and at $\rho \ll z$ (Ref. 14):

$$\Phi_{mk}^{\text{Coul}}(\mathbf{r}) \approx \Psi_{mk}^{\text{Coul}}(\mathbf{r}) + [\Psi_{mk}^{\text{Coul}}(\mathbf{r})]^*, \quad (11)$$

$$\Psi_{mk}^{\text{Coul}}(\mathbf{r}) = \frac{|m|! e^{im\varphi}}{2(\pi z p)^{1/2}} \left(\frac{\rho^2}{2\alpha z} \right)^{|m|/2} L_k^{|m|} \left(\frac{\kappa \rho^2}{2z} \right)$$

$$\times \exp \left[i \int_0^z \left(p - \frac{\kappa(2k+|m|+1)}{2zp} \right) dz - \frac{\kappa \rho^2}{4z} - \frac{i\pi}{4} (2m+1) \right]. \quad (12)$$

It is easy to verify that the wave function $\Psi_{mk}(\mathbf{r})$ coincides with (12) if we put in (9) $a_{11} = a_{22}^{-1} = \kappa/\alpha$ and $a_{12} = 0$. This joining, however, fixes all the free parameters a_{ij} of the matrix \mathbf{A} , which should remain arbitrary so far and should be determined by the quantization rule. At arbitrary a_{ij} , the solution (9) is joined to a linear combination of the functions Ψ_m^{Coul} ($l = 0, 1, 2, \dots$):

$$\Psi_{mk}(\mathbf{r}) = \sum_{l=0}^{\infty} C_{mkl} \Psi_{ml}^{\text{Coul}}(\mathbf{r}). \quad (13)$$

We shall be interested hereafter only in the case $a_{12} = 0$ (see (15)). We then obtain for the Fourier coefficients C_{mkl}

$$C_{mkl} = \frac{(2\pi)^{1/2} (k+|m|)!}{2(|m|!)^2 k!} \times \exp \left[i\pi \left(k + \frac{m}{2} + \frac{1}{4} \right) \right] \frac{\alpha^{|m|+1/2}}{a_{22}^{(|m|+1)/2}} (1-s)^{|m|+1} s^{k+1} \times F \left(-k, -l; |m|+1; 1 - \frac{1}{s^2} \right), \quad s = \frac{\alpha - \kappa a_{22}}{\alpha + \kappa a_{22}}, \quad (14)$$

where $F(a, b; c; x)$ is a hypergeometric function that can be expressed in elementary fashion in terms of a Jacobi polynomial. We now replace Ψ_{ml}^{Coul} in (13) by the function $(\Psi_{ml}^{\text{Coul}})^*$ [see (11)] and again sum this expression over a formula similar to (13). As a result we find that an exponential decrease as $z \rightarrow -\infty$ is given by a linear combination of $\Psi_{mk} \rightarrow \Psi_{mk}^*$, where Ψ_{mk}^* is a function formally conjugate to Ψ_{mk} (i.e., it is necessary to replace i in (9) by $-i$), in which a_{12} is replaced by $-a_{12}$ in expression (19) for $\sigma(z)$.

Near the turning point z_1 , where the solution (9), being quasiclassical in z , no longer holds, the joining can be effected by the standard-problem method.¹³ It is found in the upshot that, in analogy with the one-dimensional Jeffries rule, when the wave (9) is reflected from z_1 it is replaced by its formal conjugate multiplied by $\exp(i\pi/2)$. In addition, the off-diagonal elements of the matrix $\mathbf{T}^{\dagger} \mathbf{A} \mathbf{T}$ (\dagger denotes the transpose), which like \mathbf{A} is symmetrical, reverse sign.

Thus, upon "reflection" of the wave (9) from the center and from the turning point z_1 , the off-diagonal elements of the matrices \mathbf{A} and $\mathbf{A}^{\dagger} \mathbf{T} \mathbf{A}$, respectively, reverse sign. The requirement that a wave function go over into itself after two reflections [that the solution have in the classically allowed region the form $\cos(\dots)$] leads to the condition that the indicated matrices be diagonal:

$$a_{11} = a_{22}^{-1} = (-t_{22} t_{21} / t_{11} t_{12})^{1/2}, \quad a_{12} = a_{21} = 0, \quad (15)$$

and to the quantization rule

$$\int_0^{z_1} [2(E_{mnk} - V^0(z))]^{1/2} dz = n\pi + (2k+|m|+1) \arctg \left(-\frac{t_{21} t_{12}}{t_{11} t_{22}} \right)^{1/2}; \quad (16)$$

$n \gg 2k + |m| + 1; k \gg 0; n$ and k are integers. It is shown in Appendix 1 that a positive radicand in (16) is equivalent to the condition for the stability of the trajectory $\rho = 0$ in phase space. As seen from (16), the degeneracy of the levels E_{mnk} in k and m is preserved in the approximation considered.

As a result we obtain in the region $z \gg \rho$ the following expression for the normalized eigenfunctions:

$$\Psi_{mnk} = \frac{(2k!)^{1/2}}{[\pi(k+|m|)!]^{1/2}} \left(\int_0^{z_1} \frac{dz}{p} \right)^{-1/2} (\Psi_{mk} + \Psi_{mk}^*)|_{z=E_{mnk}}. \quad (17)$$

This equation does not hold in a small vicinity of the atomic center, where $z \sim n(2k + |m| + 1/\alpha)$. In this region the eigenfunctions are determined by Eqs. (13) and (14) at $E = E_{mnk}$ and go over into (17) at $z \gg \rho$ and $z \gg \alpha^{-1}$.

If the perturbation $W(z, \rho)$ is symmetric about z (as in the case of a hydrogen atom in a magnetic field), the correct wave functions are given by

$$\Psi_{mnk}^{\pm}(z, \rho, \varphi) = 2^{-1/2} (\Psi_{mnk}(z, \rho, \varphi) + \Psi_{mnk}(-z, \rho, \varphi)). \quad (18)$$

The levels E_{mnk} are in this approximation additionally doubly degenerate in parity, inasmuch as in determining the eigenfunctions Ψ_{mnk} we have neglected the interaction W where the functions Ψ_{mnk} are exponentially small. Allowance for W in this region leads to an exponentially small level splitting, which is not considered in the present paper.

3. HYDROGEN ATOM IN A MAGNETIC FIELD

The potential (2) for a hydrogen atom in a magnetic field can be represented in the form

$$V(z, \rho) = -\frac{\alpha}{z} + \rho^2 \left(\frac{\alpha}{2z^3} + \frac{\gamma^2}{8} \right), \quad \gamma = \frac{B}{B_0}, \quad B_0 = 2.35 \cdot 10^5 \text{ T}. \quad (19)$$

We have left out here a trivial paramagnetic term. We introduce the dimensionless coordinate $\xi = \kappa^2 z / 2\alpha$ and the dimensionless parameter $\omega = \gamma^2 \alpha^2 / \kappa^6$. Equation (4) is then transformed into

$$\xi^2 (1-\xi)^2 y_{\xi\xi} + [s/16 + \omega \xi^3 (1-\xi)] y = 0. \quad (20)$$

We shall consider the cases of weak ($\omega \ll 1$) and strong ($\omega \gg 1$) magnetic fields.

a. At $\omega \ll 1$ Eq. (20) can be solved by iteration. The result in first order in ω is

$$\mathbf{T} = \begin{pmatrix} \frac{2\alpha}{\kappa^2} \left(1 - \frac{2\omega}{3} \right) & -\frac{5\pi\kappa\omega}{16} \\ \frac{\pi\omega}{4\kappa} & \frac{\kappa^2}{2\alpha} \left(1 + \frac{2\omega}{3} \right) \end{pmatrix}. \quad (21)$$

From (21) follows directly stability of the symmetry axis for small ω . Thus, using the results of the preceding section, we arrive at a formula for the energy levels¹⁾:

$$E_{mnk}^1 = -\frac{\alpha^2}{2n^2} + (2k+|m|+1) \frac{\sqrt{5n^3} \gamma^2}{8\alpha^2} \quad (22)$$

and at an expression for the constants in the expansion (13), (14):

$$a_{22} = a_{11}^{-1} = \sqrt{5}n(1 - 2\omega/3),$$

$$s = [(1 - \sqrt{5}) / (1 + \sqrt{5})] (1 - \sqrt{5}\omega/3). \quad (23)$$

As $\omega \rightarrow 0$ this equation determines together with (13) and (14) the correct zeroth approximation for the wave function of a hydrogen atom in a magnetic field. The degeneracy of the unperturbed Coulomb problem manifests itself in our case in the fact that in the zeroth approximation in ω the matrix \mathbf{T} is diagonal [see (21)] and an indeterminacy of type 0/0 arises, according to (15), when the constants a_{ii} are determined by perturbation theory.

Obviously, the smaller s in (14) the faster the convergence of the expansion (13) and consequently the closer the system considered to a system with separable variables. For a hydrogen atom in a constant electric field it can be easily found that $s = 0$ in the zeroth approximation, and the sum (13) consists of only one term. For the considered case of a magnetic field, the value of s in the zeroth approximation equals 0.382 according to (23).

b. To solve Eq. (20) at large ω , we obtain first the solutions of this equation in the region $\omega \zeta^3 \gg 1$ by the WKB method, and then join them with the solutions, expressed in terms of Bessel functions, at $\zeta \ll 1$. As a result we obtain the uniform asymptotes y_1 and y_2 at $\omega \gg 1$:

$$y_1 = \frac{\Gamma(1/6) \alpha \zeta^{1/2}}{3^{1/6} \omega^{1/2}} J_{1/6}(u), \quad y_2 = -\frac{2\Gamma(5/6) \omega^{1/2} \zeta^{1/2}}{3^{1/6} \omega^{1/2}} J_{-1/6}(u),$$

$$u = \omega^{1/2} \int_0^{\zeta} \frac{\zeta^{1/2}}{(1-\zeta)^{1/2}} d\zeta, \quad (24)$$

where $J_\nu(u)$ is a Bessel function, whence

$$\mathbf{T} = \begin{pmatrix} \frac{\Gamma(1/6) \alpha}{\pi^{1/2} (3\omega)^{1/2} \omega^{1/2}} \cos\left(\frac{\pi\omega^{1/2}}{2} - \frac{\pi}{3}\right) & -\frac{\Gamma(1/6) \omega^{1/2} \alpha}{2 \cdot 3^{1/6} \pi^{1/2}} \sin\left(\frac{\pi\omega^{1/2}}{2} - \frac{\pi}{3}\right) \\ -\frac{2 \cdot 3^{1/6} \Gamma(1/6)}{\pi^{1/2} \omega^{1/2} \alpha} \sin\left(\frac{\pi\omega^{1/2}}{2} + \frac{\pi}{3}\right) & -\frac{\Gamma(1/6) (3\omega)^{1/2} \alpha^2}{\alpha \sqrt{\pi}} \cos\left(\frac{\pi\omega^{1/2}}{2} + \frac{\pi}{3}\right) \end{pmatrix} \quad (25)$$

and the quantization rule (16) takes the form

$$\frac{\alpha\pi}{\kappa} = n\pi + (2k + |m| + 1) \times \arctg \left[\operatorname{tg} \left(\frac{\pi\omega^{1/2}}{2} + \frac{\pi}{3} \right) \operatorname{tg} \left(\frac{\pi\omega^{1/2}}{2} - \frac{\pi}{3} \right) \right]^{1/2}. \quad (26)$$

It can be seen from this equation that when the magnetic field is varied the trajectory lying on the symmetry axis of the potential loses and regains stability periodically. The regions of stability, or of the positiveness of the radicand in (26), are determined by the condition

$$\omega_q^- < \omega < \omega_q^+, \quad (\omega_q^\pm)^{1/2} = q + 1/2 \pm 1/\epsilon, \quad (27)$$

where $q \gg 1$ and is an integer. The values $\omega = \omega_q^\pm$ coincide with the classical resonances (see Appendix 1). Assume, e.g., $n = 100$, $q = 10, 11, 12, \dots$, and $\alpha = 1$. The magnetic field corresponding to ω_q^+ runs through then to the values 2.51, 2.74, 2.98, ..., T . At the boundaries of the stability bands the

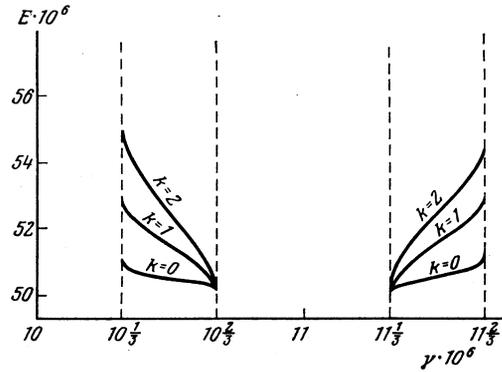


Fig. 1. Behavior of the terms in the stability bands at $n = 100$ and $m = 0$.

arctangent in (26) is equal to zero or to $\pi/2$. In this case, as can be seen from (26), additional level degeneracy is possible. If, for example, the arctangent at $\omega = \omega_q^\pm$ is zero, at fixed m and n the terms corresponding to different quantum numbers k come closer together, then at fixed m and n , when the magnetic field γ comes closer to the values $\alpha^2(\omega_q^\pm)^{1/2}/n^3$ the terms corresponding to different quantum numbers k come closer together (see Fig. 1). In the immediate vicinity of these "pseudocrossings" the quasiclassical approximation no longer holds, and a quantum approach is essential. The vicinities of ω_q^\pm where the approximation used in the present paper becomes invalid are indicated in Appendix 2.

The approximation of the potential in a region around the atomic center with a radius of the order of $n(2k + |m| + 1)/\alpha$ by a pure Coulomb potential, an approximation which we used when joining the solutions in Sec. 1, as well as the condition that the transverse momentum be small, impose an upper bound on the magnetic field, so that the quantization rule (20) is valid at

$$n/(2k + |m| + 1) \gg \omega^{1/2} \gg 1. \quad (28)$$

The phase $\pi/3$ appears in (26) because of the interaction of the degrees of freedom in the region where the variables are not separable, i.e., where the terms in the parentheses in the expression (19) for the potential are of the same order. The influence of this interaction on the quantization rule is appreciable in a sufficiently strong magnetic field and at a sufficiently large quantum number n , and under the condition (28) the levels (26) do not include the Landau levels. In order that the second term in the right-hand side of (26) describe harmonic-oscillator levels it is obviously necessary to replace the phases $\pi/3$ by zeros.

The quantization rule (26) can be solved by iteration under the condition (28). We then obtain in first order in the perturbation of the Coulomb spectrum:

$$E_{mns} = -\frac{\alpha}{2n^2} + \frac{2(2k + |m| + 1)}{\pi n^3} \arctg \left[\operatorname{tg} \left(\frac{\pi n^3 \gamma}{2\alpha^2} + \frac{\pi}{3} \right) \operatorname{tg} \left(\frac{\pi n^3 \gamma}{2\alpha^2} - \frac{\pi}{3} \right) \right]^{1/2}. \quad (29)$$

The stability condition (27) takes the form

$$\gamma_{nq}^- < \gamma < \gamma_{nq}^+, \quad \gamma_{nq}^\pm = \alpha^2 n^{-3} \left(q + \frac{1}{2} \pm \frac{1}{6} \right). \quad (30)$$

4. HYDROGEN ATOM IN PARALLEL ELECTRIC AND MAGNETIC FIELDS

The phenomenon connected with the loss of stability of the symmetry axis is observed also for a hydrogen atom in parallel electric and magnetic fields, which can furthermore be relatively weak. Assume that an electric field $\mathcal{E}z$ has been added to the potential (19):

$$V(z, \rho) = -\frac{\alpha}{z} + \mathcal{E}z + \rho^2 \left(\frac{\alpha}{2z^3} + \frac{\gamma^2}{8} \right). \quad (32)$$

The matrix \mathbf{T} has in this case, in first order in γ^2 and \mathcal{E} , the form

$$\mathbf{T} = \begin{pmatrix} \frac{2\alpha}{\kappa^2} \left(1 - \frac{2\omega}{3} \right) & -\frac{\pi\kappa}{16} (5\omega - 3\epsilon) \\ \frac{\pi}{4\kappa} (\omega - 3\epsilon) & \frac{\kappa^2}{2\alpha} \left(1 + \frac{2\omega}{3} \right) \end{pmatrix}, \quad (33)$$

$$\epsilon = \frac{4\alpha\mathcal{E}}{\kappa^4}, \quad \omega = \frac{\gamma^2\alpha^2}{\kappa^6},$$

from which we obtain an expression for the energy levels²⁾:

$$E_{mnk} = -\frac{\alpha^2}{2n^2} - \frac{3}{2} \frac{\mathcal{E}}{\alpha} n^2 + \frac{(2k + |m| + 1)}{2\alpha} \times \left[\left(\frac{5\gamma^2 n^2}{4\alpha} - 3\mathcal{E} \right) \left(\frac{\gamma^2 n^2}{4\alpha} - 3\mathcal{E} \right) \right]^{1/2}. \quad (34)$$

At $\gamma = 0$ Eq. (34) is exactly the formula for the linear Stark effect for the hydrogen atom.¹⁵ The cause of this remarkable result is that in first order in \mathcal{E} the level shift is linear in the difference between the parabolic quantum numbers.

For the considered eigenfunctions to exist it is necessary to satisfy the condition for the stability of the trajectory $\rho = 0$ [which is equivalent to the condition that the radicand in (34) be positive]:

$$\mathcal{E}\alpha/\gamma^2 n^2 > 5/12 \quad \text{or} \quad \mathcal{E}\alpha/\gamma^2 n^2 < 1/12. \quad (35)$$

It can be seen from (34) that, just as in the strong-magnetic-field case considered in the preceding section, terms with different $2k + |m| + 1$ come closer together when the boundaries of the stability regions (35) are approached. The corresponding wave functions become smeared out with respect to ρ , and the method employed is no longer valid. It is shown in Appendix 2 that the region where the method is valid is determined by condition (A7).

We consider now the case of a strong magnetic field, $\omega \gg 1$, and a moderate electric field, $\epsilon \lesssim 1$. In this case, in analogy with the preceding section, the WKB method can yield uniform asymptotic solutions of Eq. (4). As a result we arrive at the quantization rule

$$\frac{4\alpha}{3\kappa} Q(\epsilon) = \pi n + (2k + |m| + 1) \times \arctg \left[\operatorname{tg} \left(\omega^{1/2} P(\epsilon) + \frac{\pi}{3} \right) \operatorname{tg} \left(\omega^{1/2} P(\epsilon) - \frac{\pi}{3} \right) \right]^{1/2}, \quad (36)$$

$$Q(\epsilon) = \epsilon^{-1/4} (2/\beta)^{1/2} [2E(\beta) - (1-4\epsilon)^{1/2} K(\beta)], \quad (37)$$

$$P(\epsilon) = 2\epsilon^{-1/4} (2/\beta)^{1/2} [K(\beta) - E(\beta)], \quad \beta = 2\epsilon^{1/2} / [1 + (1-4\epsilon)^{1/2}],$$

where $E(\beta)$ and $K(\beta)$ are complete elliptic integrals of the first and second kind. As $\epsilon \rightarrow 0$, Eq. (36) goes over into (26). The stability bands are determined from (36) by using a formula similar to (27):

$$\omega_q^-(\epsilon) < \omega < \omega_q^+(\epsilon), \quad [\omega_q^\pm(\epsilon)]^{1/2} = (\pi/P(\epsilon)) (q + 1/2 \pm 1/\epsilon), \quad (38)$$

where $q \gg 1$ and is an integer.

5. DIPOLE MATRIX ELEMENTS

Although the expression obtained in Sec. 2 for the electron eigenfunctions is quite cumbersome, it can be used to derive simple analytic expressions for the dipole matrix elements. They are obtained below for transitions from the ground state into a highly excited one (m, n, k). The calculation of the dipole matrix elements

$$\langle \Psi_0 | \mathbf{r} | \Psi_{mnk} \rangle, \quad \Psi_0 = \alpha^{3/2} \pi^{-1/2} e^{-\alpha r/2}, \quad (39)$$

reduces in fact to integrals with the Coulomb functions, since the low-lying states, and in particular the ground state Ψ_0 , are concentrated near the center, where the external field can be neglected. From (13) and (17) we have

$$\langle \Psi_0 | z | \Psi_{mnk} \rangle = \frac{(2k!)^{1/2}}{[\pi(k+|m|)!]^{1/2}} \left(\int_0^{z_1} \frac{dz}{p} \right)^{-1/2} \times \sum_{l=0}^{\infty} C_{mkl} \langle \Psi_0 | z | \Phi_{mnl}^{\text{Coul}} \rangle, \quad (40)$$

where Φ_{mnl}^{Coul} is defined by Eq. (8) with $E = E_{mnl}$, while C_{mkl} is defined by Eqs. (14). According to the selection rules, a nonzero value of the matrix elements in (39) is obtained only at $m = 0$ and ± 1 . Calculating the integrals in (40) by using the formulas of §f in Ref. 15, we find

$$\langle \Psi_0 | z | \Psi_{0nk} \rangle = \frac{(-1)^{k+1} 16\pi^{1/2}}{e^2 \alpha^2 a_{22}^{1/2}} \left(\int_0^{z_1} \frac{dz}{p} \right)^{-1/2} (1-s)^{s^k} \times \sum_{l=0}^{\infty} s^l F \left(-k, -l; 1; 1 - \frac{1}{s^2} \right). \quad (41)$$

Calculating the sum in (41) in accord with Ref. 14 we obtain ultimately

$$|\langle \Psi_0 | z | \Psi_{0nk} \rangle|^2 = \frac{2^8 \pi}{e^4 \alpha^4 a_{22}^2} \left(\int_0^{z_1} \frac{dz}{p} \right)^{-1}, \quad a_{22} = \left(-\frac{t_{11} t_{12}}{t_{22} t_{21}} \right)^{1/2}. \quad (42)$$

We obtain analogously an expression for the oscillator strengths in the case of transverse polarization ($m = \pm 1$):

$$|\langle \Psi_0 | x | \Psi_{\pm 1nk} \rangle|^2 = \frac{2^8 \pi (k+1)}{e^4 \alpha^4 a_{22}^2} \left(\int_0^{z_1} \frac{dz}{p} \right)^{-1}. \quad (43)$$

For a hydrogen atom in a weak electric field we have $\alpha = 1$, $a_{22} = n$, the integral in (42) and (43) is equal to πn^3 , and k coincides with the parabolic quantum number. Equations (42) and (43) coincide then with the asymptotic forms, as $n \rightarrow \infty$, of the expressions for the oscillator strengths.¹¹

We consider now a hydrogen atom in a magnetic field. In this case the wave functions, according to (18), are doubly degenerate in parity. Transitions are allowed to odd states in

the case of longitudinal polarization and to even ones in the transverse case. The corresponding oscillator strengths will obviously be double those of (42) and (43).

For a weak magnetic field ($\omega \ll 1$), using expression (21) for the matrix \mathbf{T} , we obtain

$$|\langle \Psi_0 | z | \Psi_{\pm n}^- \rangle|^2 = \frac{2^3(1+2\omega-3)}{5e^2\alpha^2 n^2}; \quad (44)$$

$$|\langle \Psi_0 | x | \Psi_{\pm n}^- \rangle|^2 = \frac{2^2(k+1)(1-4\omega-3)}{5e^2\alpha^2 n^2}. \quad (45)$$

As $\omega \rightarrow 0$, these equations differ only by constant factors from the asymptotic (as $n \rightarrow \infty$) matrix elements on the parabolic wave functions.¹¹ The oscillator strengths for the transitions into the states under consideration are maximal for longitudinal polarization of the radiation and minimal for transverse. In Fig. 2 are compared the oscillator strengths obtained from (44) ($m=0$) with the results of a numerical calculation³ for a magnetic field of 4.7 T ($\gamma = 2 \times 10^{-5}$) using 1500 basis functions. The agreement is very good up to $n=37$ ($\omega \ll 1$).

In the case of a strong magnetic field ($\omega \gg 1$) we use the value of the matrix \mathbf{T} (25). As a result we obtain for the transition from the ground state Ψ_0 to a highly excited state with $m=0$, according to (43)

$$|\langle \Psi_0 | z | \Psi_{\pm n}^- \rangle|^2 = \frac{2^{11} 3^{1/2} \pi^{1/2} \alpha^{1/2} b^{1/2}}{e^2 \Gamma^2(1/2) n^2}, \quad b = \frac{\sin(\pi\omega^{1/2} - 2\pi/3)}{\sin(\pi\omega^{1/2} - 2\pi/3)}, \quad (46)$$

and for an analogous transition into a state with $m = \pm 1$

$$|\langle \Psi_0 | x | \Psi_{\pm n}^+ \rangle|^2 = \frac{2^{13} 3^{1/2} \pi^{1/2} (k+1) \alpha^{1/2} \gamma^{1/2} b}{e^2 \Gamma^2(1/2) n^2}. \quad (47)$$

Equations (46) and (47) show that the oscillator strengths oscillate with changing magnetic field (as well as at fixed γ with changing n). Oscillator strengths were numerically obtained in Ref. 3 at $\gamma = 2 \times 10^{-5}$ and $n = 16, \dots, 50$ (in this case $\omega^{1/2} \approx \gamma n^3 \ll 2.5$). The dependence of the oscillator strengths on n , according to Ref. 3, likewise ceases to be monotonic in the tail of the investigated spectrum following after a strong mixing at $\gamma n^3 \sim 1$. The results (46) and (47) correspond to the case $\gamma n^3 \gg 1$ and describe the behavior of the oscillator strengths in the stability zones. Although the parameter $\omega^{1/2}$

is not large enough for the states considered in Ref. 3, Fig. 2 shows a comparison of the oscillator strengths in the case $m=0$ in the stability zones corresponding, according to (27), to $n=41, 42, 43$ and $n=49, 50, 51$.

At the boundary of the stability bands, at $\omega = \omega_q^-$, expressions (46) and (47) have a singularity due to the decay of the states considered, and at $\omega = \omega_q^-$ it vanishes. The relative increase of the radiation intensity near ω_q^- is determined by the factor $b^{1/2}$ for $m=0$ and by the factor b for $m = \pm 1$. Near resonance we have

$$b \approx (3\omega)^{-1/2} \pi |\omega - \omega_q^-|. \quad (48)$$

Equation (48) is valid under the conditions (A5) and (2.6) of Appendix 2. The maximum value of b can be estimated by putting, according to (A8), $\omega - \omega_q^- \approx \omega^{1/2}/n^2$, whence $b \leq n^2$.

We present, finally, expressions for the oscillator strengths in the case of a hydrogen atom in weak parallel electric and magnetic fields. They are obtained in elementary fashion from Eqs. (42), (43), and (33):

$$|\langle \Psi_0 | z | \Psi_{\pm n k} \rangle|^2 = \frac{2^5}{(e\alpha n)^2} \left(\frac{\omega - 3\varepsilon}{5\omega - 3\varepsilon} \right)^{1/2}, \quad (49)$$

$$|\langle \Psi_0 | x | \Psi_{\pm n k} \rangle|^2 = 2^5 (k+1) (\omega - 3\varepsilon) / (e\alpha)^2 n^5 (5\omega - 3\varepsilon). \quad (50)$$

It can be seen that near the boundaries of the stability zones we have here, too, either a spike or a dip of the radiation intensity.

We note in conclusion that the symmetry plane $z=0$ possessed by the hydrogen atom in a magnetic field goes over, after separating the azimuthal factor $\exp(im\varphi)$ in the Schrödinger equation, into a symmetry axis in the (z, ρ) plane. The natural oscillations in the vicinity of the $z=0$ plane were considered in a number of papers (see Ref. 4 and the literature cited there). They can also be investigated by the method proposed in the present paper. In particular, the corresponding quantization rule for large m is contained in Ref. 16.

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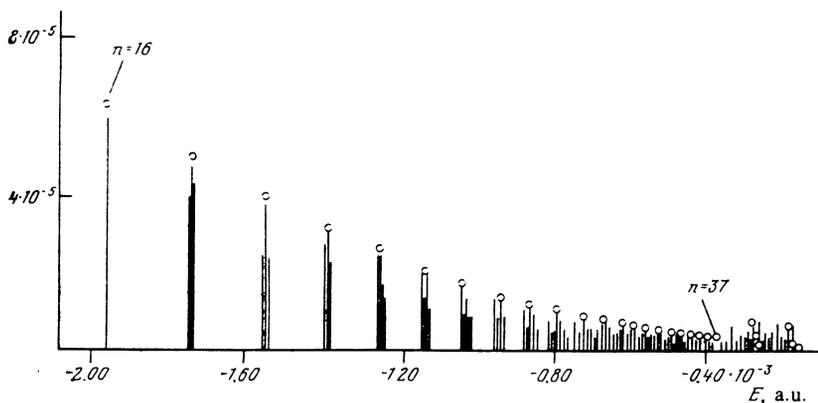


Fig. 2. Comparison of the oscillator strengths calculated by Eq. (44) (points, $n \leq 37$) with the numerical calculation.³ The last six points were calculated from Eq. (46) in the stability bands.

APPENDIX 1

We derive the equations from the classical trajectories (3). To this end we substitute the function $\rho(z)$ in the initial Newton's equations

$$\ddot{z} = -\partial V/\partial z, \quad \ddot{\rho} = -\partial V/\partial \rho,$$

and eliminate the time derivative, making use of the energy integral. As a result we obtain for the function $\rho(z)$ the equation

$$\rho_{zz} \frac{2(E-V)}{1+\rho^2} - \rho_z \frac{\partial V}{\partial z} + \frac{\partial V}{\partial \rho} = 0.$$

Assuming ρ and ρ_z to be small quantities, and also using the expression (2) for the potential at small ρ , we linearize this equation with respect to ρ . As a result we arrive at (3).

Since the motion described by Eq. (13) [or (4)] is finite and is contained in the interval $(0, z_1)$, these equations can be regarded as periodic with a period $2z_1$ on the entire z axis. We can then determine the constant monodromy matrix¹² that connects the solutions on the interval $(0, 2z_1)$ with the solutions on the interval $(2qz_1, 2(q+1)z_1)$ (i.e., after q reflections from z_1), using the formula

$$y(z+2qz_1) = B^q y(z).$$

It is known that the determinant of the monodromy matrix B is equal to unity. Its eigenvalue can therefore be represented in the form

$$\lambda_1 = e^{i\mu}, \quad \lambda_2 = e^{-i\mu}.$$

The quantity μ is called the characteristic exponent. It can be easily shown that the z axis is stable if the matrix B can be diagonalized by a nonsingular transformation $Q^{-1}BQ$ and if μ is real. This condition is also necessary for stability. It is obvious that if the characteristic exponent is equal to a rational fraction of π ($\mu = p\pi/q$), all the trajectories are closed after q reflections from z_1 . In particular, at $\mu = 0$ all the trajectories are closed after one revolution. Thus, resonance sets in after $\mu = p\pi/q$ (Ref. 17).

The monodromy matrix is expressed in elementary fashion in terms of the matrix T introduced in Sec. 1:

$$B = JT^{-1}JT, \quad J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (A1)$$

To obtain this equation it suffices to note that the solutions y_2^1 (6) and y_2^0 (5) reverse sign after reflection from z_1 and rotation around the center, respectively, and the solutions y_1^1 and y_1^0 remain unchanged. From (A1) we obtain

$$\mu = 2 \arctg \left(-t_{12}t_{21}/t_{11}t_{22} \right)^{1/2}. \quad (A2)$$

This is just the expression contained in the quantization rule (16).

APPENDIX 2

The approximation considered is not valid in the immediate vicinity of the boundaries of stability zones, since the wave functions are smeared out here with respect to ρ . The characteristic width of the wave function, according to (9), is estimated at

$$\rho_0 \sim \sigma p^{-1/2} (2k + |m| + 1)^{1/2} \ll n^2/\alpha. \quad (A3)$$

The inequality in (A3) means that ρ_0 should be much less

than the characteristic quantity $z \sim n^2/\alpha$. In a weak field $\sigma^2 \sim zp/\kappa$ and (A3) is equivalent to the condition $2k + |m| + 1 \ll n$.

In a strong magnetic field, at $\omega \zeta^3 \gg 1$, the quantity $\sigma(z)$ is defined by the equation

$$\sigma^2(z) = \frac{4\alpha}{\kappa^2 (\omega \zeta)^{1/2}} \left[\left(\frac{\sin(\pi\omega^{1/2} + 2\pi/3)}{\sin(\pi\omega^{1/2} - 2\pi/3)} \right)^{1/2} \cos^2 \left(u - \frac{\pi}{3} \right) + \left(\frac{\sin(\pi\omega^{1/2} - 2\pi/3)}{\sin(\pi\omega^{1/2} + 2\pi/3)} \right)^{1/2} \sin^2 \left(u + \frac{\pi}{3} \right) \right], \quad u = \omega^{1/2} \int_0^z \frac{d\xi \zeta^{1/2}}{(1-\xi)^{1/2}}. \quad (A4)$$

If ω is not close to ω_q^\pm , we have $\sigma^2 \sim \alpha \kappa^{-2}/(\omega \zeta)^{1/2}$ and the condition (A3) is satisfied at $k, m \ll n$. Near ω_q^\pm the z axis has nodal points determined by the zeros of the cosines in (A4), where the wave function is possibly not smeared. Outside the nodal points, at ω close to ω_q^\pm , the width of the wave function is

$$\rho_0 \sim n^{3/2} (2k + |m| + 1)^{1/2} / \alpha \omega^{1/4} |\omega - \omega_q^\pm|^{1/4}$$

and the condition (A3) can be rewritten in the form

$$|\omega - \omega_q^\pm| \gg (2k + |m| + 1)^2 / n^2 \omega^{1/2}. \quad (A5)$$

For a hydrogen atom in weak parallel electric and magnetic fields we obtain for $\sigma(z)$ in the zeroth approximation in the field

$$\sigma^2(z) \approx \frac{4\alpha}{\kappa^2} [\xi(1-\xi)]^{1/2} \times \left[\left(\frac{\omega - 3\varepsilon}{5\omega - 3\varepsilon} \right)^{1/2} \xi + \left(\frac{5\omega - 3\varepsilon}{\omega - 3\varepsilon} \right)^{1/2} (1-\xi) \right]. \quad (A6)$$

Let, for example, $1 - 3\varepsilon/\omega \ll 1$. The main contribution to (A6) is then made by the second term in the square brackets (we assume that $1 - \xi \sim 1$), and we have for the characteristic width of the wave function

$$\rho_0 \sim n^{3/2} (2k + |m| + 1)^{1/2} \omega^{1/4} / \alpha (\omega - 3\varepsilon)^{1/4}.$$

Thus, according to (A3), the method considered is valid under the condition

$$\left[\left(1 - \frac{3\varepsilon}{\omega} \right) \left(1 - \frac{3\varepsilon}{5\omega} \right) \right]^{1/2} \gg \frac{2k + |m| + 1}{n}. \quad (A7)$$

We have taken into account here also the case $5 - 3\varepsilon/\omega \ll 1$.

For a hydrogen atom in a strong magnetic field, the approximation considered is generally speaking correct when $\mu \gg 1/n$ and $|\mu - \pi| \gg 1/n$ [see (A2) and (26)], where $1/n$ is the quasiclassical error of the quantization rule. These restrictions lead to the condition

$$|\omega - \omega_q^\pm|^{1/2} \gg \omega^{1/4}/n, \quad (A8)$$

which are stronger than (A5) at $k \sim 1$ and $m \sim 1$.

¹¹Here and elsewhere we omit the paramagnetic term γm that is linear in the field.

¹²A correction was introduced here for a numerical error incurred in Ref. 10.

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