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Fermi-like resonances for circular Rydberg states of a hydrogen atom in a magnetic field

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Abstract. The energy spectrum of Rydberg states of large angular momentum and relatively small value of n-|m| in an arbitrary magnetic field is calculated by the semiclassical expansion in powers of 1/|m|. The problem is approximated by an anisotropic two-dimensional harmonic oscillator. The anharmonic corrections to the energy are calculated, and the series is summed. Special emphasis is put on excited degenerate states of the harmonic oscillator (similar to Fermi resonances in a molecular vibration theory) when the 1/|m|-expansion fails to converge. Using the fact that the sum and the product of the energies of degenerate states have regular expansions, the quasi-crossings of the levels are obtained. The complex branch points joining the levels are also found.

Text

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1. Introduction

A circular Rydberg state is a state with a large magnetic quantum number m and a relatively small value of n-|m|, where n is a principal quantum number. Inside a large-|m| azimuthal subspace, it may be a ground state or one of the lowest excited states. In a such quasiclassical system, an electron moves along the circular orbit performing small vibrations both in the radial direction and in the direction orthogonal to the plane of the orbit. The vibrations are the weaker, the smaller is a value of n-|m|.

The term "circular states" is used mostly for the states with a maximum possible m (|m| = n - 1), when the oscillations around the circular trajectory have purely quantum nature. These states can be prepared by the adiabatic microwave transfer method (Hulet and Kleppner, 1983). The experiments of Liang *et al* (1986) demonstrate the feasibility of circular state spectroscopy.

Rydberg states of atomic hydrogen in a magnetic field were extensively studied from various points of view (for references, see Kleppner *et al* 1983). Zimmerman *et al* (1980) calculated the energy levels of m=0 states as functions of the magnetic field intensity. Their results display clear repulsions between numerous levels. Wunner *et al* (1986) computed the energies of circular states in a magnetic field. Here, we continue to study such high-|m| Rydberg states paying attention to level crossings.

Since the radius of the orbit rises proportionally to m^2 , the circular states are highly sensitive to diamagnetic interaction. So, the quadratic Zeeman shift may be comparable with the line spacing, and quasi-crossings occur. The object for our study is the pattern of the energy levels which exhibits regular series of quasi-crossings. Using a similarity between this problem and the spectrum of molecular vibrations, the quasicrossings are identified as Fermi resonances. The energies and complex branch points are calculated by the semiclassical method of 1/|m|-expansion applied previously for the ground state and for the states with n = |m|+1 by Bender, Mlodinow and Papanicolaou (1982).

To solve the problem, we use Rayleigh - Schrödinger perturbation theory for a two-dimensional harmonic oscillator. The eigenstates of the harmonic oscillator would be a proper zero-order approximation unless the accidental degeneracy occurs, when two or more levels corresponding to different vibrations have the same energy, and when the anharmonic corrections become infinitely large. To avoid the divergence of the perturbation theory, we use a simple trick. The resulting spectrum is shown in a whole range of magnetic field strengths.

2. The large |m| limit

The Hamiltonian of the hydrogen atom in a magnetic field **B** along *z*-axis is, in atomic units:

$$H = \frac{1}{2}p^{2} - \frac{1}{r} + \frac{B}{2}L_{z} + \frac{B^{2}}{8}(x^{2} + y^{2})$$
(1)

(atomic unity for the magnetic field is $2.35 \cdot 10^5$ T). The paramagnetic interaction $\frac{B}{2}L_z$ is an integral of motion equal $\frac{B}{2}m$, and it will be omitted further.

In cylindrical coordinates, the Schrödinger equation takes the form:

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2} + \frac{\partial^2}{\partial z^2} + \frac{1}{4\rho^2}\right) + V_{\rm eff}(\rho, z) - E\right] \Psi(\rho, z) = 0, \qquad (2)$$

where $r = (\rho^2 + z^2)^{1/2}$, and the wave function $\Psi(\mathbf{r}) = e^{im\varphi}\rho^{-1/2}\Psi(\rho,z)$. The effective potential in equation (2) is:

$$V_{\rm eff}(\rho, z) = \frac{m^2}{2\rho^2} - \frac{1}{r} + \frac{B^2}{8}\rho^2.$$
 (3)

Notice that $m^2 - 1/4$ is replaced by m^2 in the centrifugal term in V_{eff} as it is usually done in quasiclassical theory. The term $-1/4\rho^2$ remaining in the kinetic energy can be eliminated in principle by Langer transformation of the variable *r*.

Let m > 0. A convenient way to exhibit explicitly the large-*m* limit is to define rescaled variables:

$$\rho = m^2 \rho', \quad z = m^2 z', \quad E = m^{-2} E', \quad B = m^{-3} B'$$
 (4)

and assume that B' be *m* independent. Equation (2) then reads

$$\left[-\frac{1}{2m^2}\left(\frac{\partial^2}{\partial \rho'^2} + \frac{\partial^2}{\partial z'^2} + \frac{1}{4\rho'^2}\right) + V'_{\text{eff}}(\rho', z') - E'\right]\psi'(\rho', z') = 0$$
(5)

where the effective potential is

$$V'_{\rm eff}(\rho',z') = \frac{1}{2{\rho'}^2} - \frac{1}{r'} + \frac{{B'}^2}{8}{\rho'}^2.$$
(6)

Equation (5) has a form of the Schrödinger equation where 1/m plays the role of the Planck's constant, or where m^2 imitates the mass.

To solve the equation (5), we use the method from molecular vibration theory. In the large *m* limit, the wave function concentrates around the point of minimum (ρ'_0, z'_0) of the potential (6) and describe a classical particle resting on the plane (ρ', z') , the energy being $E'_0 = V'_{eff}(\rho'_0, z'_0)$. The classical limit may be regarded equally as a circular motion of a particle in a three-dimensional potential $V'(x', y', z') = -\frac{1}{r'} + \frac{B'^2}{8}\rho'^2$ with unity angular momentum along *z*-axis, the radius of the orbit being ρ'_0 and the velocity being $1/\rho'_0$.

The equilibrium coordinates are $z'_0 = 0$ and $\rho'_0 = r'_0$ where r'_0 is a positive root of an algebraic equation

$$\frac{B'^2}{4}r_0'^4 + r_0' - 1 = 0.$$
⁽⁷⁾

In a strong field limit, the equilibrium radius tends to zero. It is no longer the case after the second scaling transformation

$$\rho' = r_0' \tilde{\rho}, \quad z' = r_0' \tilde{z}, \quad E' = r_0'^{-2} \tilde{E}$$
 (8)

that yields

$$\left[-\frac{1}{2m^2}\left(\frac{\partial^2}{\partial\tilde{\rho}^2} + \frac{\partial^2}{\partial\tilde{z}^2} + \frac{1}{4\tilde{\rho}^2}\right) + \tilde{V}_{\rm eff}(\tilde{\rho},\tilde{z}) - \tilde{E}\right]\tilde{\psi}(\tilde{\rho},\tilde{z}) = 0.$$
(9)

Here,

$$\widetilde{V}_{\rm eff}(\widetilde{\rho},\widetilde{z}) = \frac{1}{2\widetilde{\rho}^2} - \frac{1-g}{\widetilde{r}} + \frac{g}{2}\widetilde{\rho}^2$$
(10)

is a new effective potential, and

$$g = B'^2 r_0'^4 / 4 = 1 - r_0' \tag{11}$$

is a coupling parameter. In the absence of field, g = 0, and the potential is purely Coulomb. In the strong field limit, g = 1, and the potential reduces to a diamagnetic term. Notice that $g^{1/4}$ coincides with the dimensionless parameter η , introduced by Bender *et al* (1982).

Since the equilibrium radius \tilde{r}_0 and the velocity $1/\tilde{r}_0$ remain unity, the classical dynamics in a potential $\tilde{V}(\tilde{x}, \tilde{y}, \tilde{z}) = -\frac{1-g}{\tilde{r}} + \frac{g}{2}\tilde{\rho}^2$ does not depend on magnetic field (for purely circular motion only, because the frequencies of vibrations still vary).

Further, we shall investigate in detail the latest scaled version of the problem because it is especially convenient for semiclassical treatment. To obtain \mathcal{G} from the given value of B', one should do successive calculation $B' \to w_1 \to w_1 \to r'_0$:

$$w_{1} = \frac{1}{2}B'^{-1/3}[1 + (1 + \frac{64}{27}B'^{2})^{1/2}]^{1/3},$$

$$w_{2} = B'^{-1/2}(w_{1} - w_{1}^{-1}/3)^{1/2},$$

$$r_{0}' = [(B'^{2}w_{2})^{-1} - w_{2}^{2}]^{1/2} - w_{2}$$

(when B' = 0, $r'_0 = 1$) and then use (11). Reverse, the initial problem can be parametrized in terms of $g: r'_0 = 1 - g$, $B' = 2g^{1/2}(1 - g)^{-2}$, and $E'_0 = (-1/2 + 3g/2)(1 - g)^{-2}$.

3. Calculation of the energy levels

Let us investigate the dependence of the scaled energy \tilde{E} on the coupling parameter g. Introducing displacement coordinates $\xi = m^{1/2}(\tilde{\rho} - 1)$ and $\eta = m^{1/2}\tilde{z}$, we treat the problem as a harmonic oscillator perturbed by the potential $U(\xi,\eta)$:

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2}\right) + \frac{\omega_1^2}{2}\xi^2 + \frac{\omega_2^2}{2}\eta^2 + U(\xi,\eta) - \varepsilon\right]\phi(\xi,\eta) = 0, \qquad (12)$$

where

$$U(\xi,\eta) = [\tilde{V}_{\text{eff}}(1+m^{-1/2}\xi,m^{-1/2}\eta) - \tilde{E}_0]m - \frac{m^{-1}}{8(1+m^{-1/2}\xi)} - \frac{1+3g}{2}\xi^2 - \frac{1-g}{2}\eta^2 = -[(1+g)\xi^3 + \frac{3}{2}(1-g)\xi\eta^2]m^{-1/2} + \left[\left(\frac{3}{2}+g\right)\xi^4 - \frac{3}{8}(1-g)\eta^4 + 3(1-g)\xi^2\eta^2 - \frac{1}{8}\right]m^{-1} + \dots, \quad (13)$$

$$\varepsilon = (\widetilde{E} - \widetilde{E}_0)m = (n_1 + 1/2)\omega_1 + (n_2 + 1/2)\omega_2 + \text{(anharmonic terms)}, \qquad (14)$$

$$\omega_1 = \sqrt{1+3g}, \quad \omega_2 = \sqrt{1-g} \tag{15}$$

are the frequencies of normal oscillations, and $\varphi(\xi,\eta) = \widetilde{\psi}(1 + m^{-1/2}\xi, m^{-1/2}\eta)$. The anharmonic terms in the energy represent a series in powers of 1/m whose coefficients are calculated from the recurrence relations previously used by Vainberg, Popov and Sergeev (1990).

For the ground state of the oscillator $(n_1 = n_2 = 0)$, this series can be easily summed for all *m*, even for $m \sim 1$. The same result was obtained by Bender *et al* (1982) who used a similar expansion in powers of 1/(m+1). The resulting curves $\tilde{E}(g)$ are shown in the Figure 1. To improve the convergence of the 1/m-series for low values of *m*, we use Padé approximants (up to the order [4/4]). The interesting fact is that these curves become almost straight lines, when m > 5. In the limit $m \to \infty$ (the lowest curve), the energy is a strictly linear function

$$\tilde{E}_0(g) = -\frac{1}{2} + \frac{3}{2}g.$$
(16)

The figure 1 gives a survey of the entire range of the field strengths from the zero field $\tilde{E}(0) = -m^2 / 2(m + n_1 + n_2 + 1)^2$ up to the infinite field limit $\tilde{E}(1) = (m + 2n_1 + 1) / m$.

Now, let us examine the excited states. Since the curves are close to the classical limit (16) when *m* is large, it is convenient to plot the vibrational part of the energy $\varepsilon(g)$ instead of the full energy $\tilde{E}(g) = \tilde{E}_0(g) + \varepsilon(g)m^{-1}$.

In the limit $m \to \infty$, the curves $\varepsilon(g) = (n_1 + 1/2)\omega_1 + (n_2 + 1/2)\omega_2$ are presented in the figure 2. When g = 0, the frequencies (15) equal to unity, and the vibrational energy ε coincides with a sum $p = n_1 + n_2 + 1$. So, the curves form the bunches corresponding to a definite principal quantum number n = m + p. In the opposite limit, $\omega_1 = 2$, $\omega_2 = 0$, $\varepsilon(1) = 2n_1 + 1$, and the curves cluster into Landau resonances. When g = 3/7, the frequencies are related as 2:1, and the series of curve-crossings can be easily traced. There is an obvious similarity between this case and well-known Fermi resonances in CO₂ molecule (Herzberg 1945).

For instance, let us consider the states (10) and (02) for $g \approx 3/7$ using a standard method of degenerate perturbation theory. Since $|10\rangle$ and $|02\rangle$ eigenstates of the harmonic oscillator have nearly the same energy and thus perturb one another, the zero-order wave function should be its linear combination. The diagonal matrix elements of the Hamiltonian in equation (12) are $|10\rangle$ and $H_{22} = \frac{1}{2}\omega_1 + \frac{5}{2}\omega_2$. The anharmonicity that mixes the oscillator's eigenstates is $u_{12}\xi\eta^2m^{-1/2}$, where the potential constant is $u_{12} = 3(g-1)/2$, see equation (13). So, off-diagonal matrix elements are:

$$H_{12} = H_{21} = u_{12}m^{-1/2} \langle 10|\xi\eta^2|02\rangle = \frac{u_{12}m^{-1/2}}{2\omega_1^{1/2}\omega_2}.$$
 (17)

Solving the secular equation

$$\begin{vmatrix} H_{11} - \varepsilon & H_{12} \\ H_{21} & H_{22} - \varepsilon \end{vmatrix} = 0,$$
(18)

one obtains the energy

$$\varepsilon = \omega_1 + \frac{3}{2}\omega_2 \pm \frac{1}{2} \left[(\omega_1 - 2\omega_2)^2 + \frac{u_{12}^2}{\omega_1 \omega_2^2} m^{-1} \right]^{1/2}.$$
 (19)

If we try to expand it into a series in powers of m^{-1} , the radius of convergence of the series would be small (it is proportional to $(\omega_1 - 2\omega_2)^2$). So, we cannot apply the 1/m-expansion directly because of its divergence.

A convenient way to overcome this difficulty is to consider the sum and the product of the energies. As their expansions have no more singularity when g = 3/7, they can be easily summed. Finally, the energies can be calculated from the corresponding quadratic equation. For the triple crossing, the energies can be computed in the same way by solution of the cubic equation.

The results of the calculation of the energy levels for m = 30 manifold are shown on figure 3. Up to eight terms of the 1/*m*-expansion were used. The limiting case g = 0corresponds to the rescaled Coulomb spectrum

$$\varepsilon(0) = p(1 + m^{-1}p/2)(1 + m^{-1}p)^{-2}$$

that is near-equidistant if $p \ll m$. When g increases, the Coulomb spectrum gradually transforms into Landau resonances $\varepsilon(1) = 2n_1 + 1$. The quasi-crossing of the levels (10) and (02) is evident; the triple (20) - (12) - (04) quasi-crossing appears to divide into a pair of (20) - (12) and (12) - (04) ordinary quasi-crossings, the separation of the levels being the same as for (10) - (02) quasi-crossing.

For (10) - (04) crossing, the separation is so small that it is invisible on the figure. Indeed, the anharmonicity that mixes the oscillator's eigenstates $|10\rangle$ and $|04\rangle$ is $u_{14}\xi\eta^4 m^{-3/2}$, where $u_{14} = 15(1-g)/8$. So, the repulsion of the levels is of the order $m^{-3/2}$ that is much less than (17) which is of the order $m^{-1/2}$. The similar no-splitting occurs for (10) - (06), (30) - (04), and for another crossings corresponding to rational values of ω_1 / ω_2 except 1/2.

The figure 4 shows the spectrum of m = 10 manifold. Here, the repulsion of the levels grows appreciably, and it is visible even for (10) - (04) quasicrossing.

Apart from the 1/*m*-expansion, it is interesting to examine applicability of the standard perturbation theory (in powers of the magnetic field squared). For this purpose, we plot on the figure 4 the curves obtained from the expansion of the energy up to the order B^6 . The analytic formulas for such an expansion for the lowest six states with $n_1 + n_2 \le 2$ are given in Appendix. The range of applicability of the perturbation theory is proved to be about g < 0.06, or $B < 0.5 m^{-3}$.

4. Branch points

When the magnetic field varies in time, the diabatic transitions between the levels occur at the points of quasi-crossings. In a quasiclassical approximation, the transition probabilities are evaluated by assuming a complex contour embracing the branch point and connecting two levels. So, it is important to establish the positions of the branch points of the energy levels in a complex plane of intensity of the magnetic field.

In the limit $m \to \infty$, the levels (n_1, n_2) and (n'_1, n'_2) cross when the ratio ω_1 / ω_2 equals to a rational number $r = (n'_2 - n_2) / (n_1 - n'_1)$, or when g reaches

$$g_{c}^{(n_{1}n_{2})-(n_{1}'n_{2}')} = (r^{2}-1)/(r^{2}+3).$$
⁽²⁰⁾

For large but finite *m*, the levels of the same parity join in branch points whose real part is given by (20), and an imaginary part is small.

Let us consider (10) and (02) states when the energies are approximated explicitly by (19). When the expression in square brackets in (19) diminishes, the energy has a square-root branch point. Expanding this expression in Taylor series around the point g = 3/7 and maintaining the terms of the order m^{-1} , one obtains the equation for the branch point g_c :

$$\frac{7}{64}(7g_c-3)^2 + \frac{9\sqrt{7}}{28}m^{-1} = 0.$$
(21)

Its solution is

$$g_c^{(10)-(02)} = \frac{3}{7} (1 \pm i \cdot 4 \cdot 7^{-3/4} m^{-1/2}).$$
(22)

For the states (11) and (03), one can similarly find

$$g_c^{(11)-(03)} = \frac{3}{7} (1 \pm i \cdot 4 \cdot 3^{1/2} \cdot 7^{-3/4} m^{-1/2})$$
(23)

To obtain the exact values of g_c , we calculate the complex roots of the function $[\varepsilon_{n_1n_2}(g) - \varepsilon_{n'_1n'_2}(g)]^2$ approximated by 1/*m*-series. The results are shown in Table 1. Here, we retain only stabile digits that do not vary when the number of terms of the 1/*m*-series grows. The results from the analytic formulas (22) and (23) are also given for comparison.

The large-*m* behavior of g_c for (10) - (04) crossing was found to be

$$g_c^{(10)-(04)} = \frac{15}{19} - 2.540m^{-1} \pm i \cdot 0.724m^{-3/2} + O(m^{-2})$$
(24)

where coefficients before m^{-1} and $m^{-3/2}$ were calculated by numerical fitting.

The branch points in the *B*-plane may be found by means of relation $B_c = 2g_c^{1/2}(1-g_c)^{-2}m^{-3}$. For instance,

$$B_c^{(10)-(02)} = \frac{7\sqrt{21}}{8}m^{-3} \pm i \cdot 7^{1/4}\sqrt{21}m^{-7/2} + O(m^{-4}).$$
⁽²⁵⁾

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So, the branch points lie closely to the real axis in complex-conjugate pairs. Their positions can be found together with the energies simply by assuming complex arithmetic.

5. Conclusion

The method of semiclassical 1/m-expansion is extended here to excited states. We consider the case when the oscillator quantum numbers n_1 and n_2 are much smaller than m, but they may be not small themselves. In our case, the typical situation is near-degeneracy of the levels because two or more excited states with different (n_1, n_2) may have approximately the same energy.

Within large-*m* framework, the quantum-mechanical problem reduces to a classical static problem and a subsequent vibrational analysis. Since near-degenerate states are highly sensitive to perturbation caused by anharmonic terms in a potential, the 1/m-expansion diverges. Suitable modification of the method is proposed that avoids the troubles related to energy quasi-crossings.

Apart from the atom in a magnetic field, the similar quasi-crossings take place for a hydrogen atom in parallel electric and magnetic fields when ω_1 / ω_2 is a rational number. The frequencies ω_1 and ω_2 as functions of rescaled field strengths $F' = m^4 F$ and $B' = m^3 B$ were obtained by Vainberg *et al* (1990). Here, we show on the figure 5 the curves on (F', B')-plane of constant ratio ω_1 / ω_2 . It should be pointed out that there are no quasi-crossings for purely electric field because of separability of the Stark problem (in parabolic coordinates).

The method of 1/m-expansion is equivalent in essence to the method of 1/D-expansion, where D is the dimensionality of coordinate space. Recently (Goodson and Watson 1993), the large-dimensional method was applied to excited states of two-electron atom corresponding to molecular-like vibrational excitations. If the charge of the nucleus assumes non-integer value $Z_c = 1.57$, then the first two frequencies of

vibrations are related as 1:2. So, one can expect near-degeneracy of the levels $(n_1 = 0, n_2 = 1)$ and $(n_1 = 2, n_2 = 0)$ for the nearest to Z_c integer charge Z = 2 corresponding to helium.

Goodson and Watson (1993) calculated the first 30 coefficients of the 1/*D*-expansion for 1s 2s ¹S state ($n_1 = 0$, $n_2 = 1$, $n_3 = 0$) and found that the 1/*D*-series is strongly divergent because of square-root singularity at 1/D = -0.0114. We explain the origin of this singularity as a result of mixing with (200) state having near the same energy, and we also propose the way to eliminate the singularity (by assuming the sum and the product of the energies).

Just recently, Germann *et al* (1995) used dimensional perturbation theory to study circular Rydberg states of the hydrogen atom in a uniform magnetic field. In contrast to their approach, the present method yields highly accurate results in the vicinity of avoided crossings. Although our results are somewhere overlapping regarding the lowest m = n-1 states, the present calculations of avoided crossings and branch points for excited states remain quite new.

Appendix. Expansions in a weak field

It is well known that the perturbation expansions for diamagnetic Zeeman effect can be derived in an analytic form both for ground and for excited states of the hydrogen atom. As for circular states, their energies up to the order B^6 were obtained by Turbiner (1984), but the terms beyond the order B^2 appear to have errors. The formulas for the states with n = |m|+1 in parallel electric and magnetic fields were found by Vainberg *et al* (1990). Here, we rewrite it putting the electric field to zero:

$$E = -\frac{1}{2n^2} + \frac{n^3}{8}(n+1)[B^2 - \frac{n^4}{48}(12n^2 + 27n + 14)B^4 + \frac{n^8}{1152}(216n^4 + 1089n^3 + 2048n^2 + 1700n + 528)B^6].$$
 (26)

The expression (26) was derived by 1/n-expansion that is equivalent to the "shifted" 1/m-expansion. Every term in (28) represent finite series in powers of 1/n. For instance, the term of the order B^4 is

$$-\frac{n^7 B^4}{384}(n+1)(12n^2+27n+14) = -\frac{B^{\prime\prime 4}}{384n^2}(12+39n^{-1}+41n^{-2}+14n^{-3}),$$

where $B'' = n^3 B$ is a rescaled magnetic field strength that is similar to B', see equation (4). So, it can be obtained *exactly* by summation of the first four terms of the 1/n-expansion.

In the similar way we have derived the formulas for the states with n = |m|+2 and n = |m|+3 corresponding in the limit $n \to \infty$ to excited states of the oscillator. Here, we present them for the first time:

$$\begin{split} \Delta E_{01} &= \frac{n^2}{8} (n^2 - 1) [B^2 - \frac{n^5}{8} (2n + 3)B^4 + \frac{n^9}{96} (18n^3 + 63n^2 + 62n + 10)B^6], \\ \Delta E_{10} &= \frac{n^2}{8} (n - 1) [(n + 5)B^2 - \frac{n^4}{24} (6n^3 + 75n^2 - 19n + 168)B^4 \\ &\quad + \frac{n^8}{144} (27n^5 + 585n^4 + 26n^3 + 3649n^2 - 1239n + 2772)B^6], \\ \Delta E_{11} &= \frac{n^2}{8} (n - 2) [(n + 5)B^2 - \frac{n^4}{16} (4n^3 + 47n^2 - 31n + 182)B^4 \\ &\quad + \frac{n^8}{384} (72n^5 + 1449n^4 - 1835n^3 + 12372n^2 - 12712n + 20856)B^6], \\ \Delta E_{20,02} &= \frac{n^2}{8} (n^2 + 3n - 7)B^2 - \frac{n^6}{128} (4n^4 + 39n^3 - 105n^2 + 199n - 238)B^4 \end{split}$$

$$+\frac{n^{10}}{3072}(72n^6+1305n^5-2877n^4+10957n^3-23250n^2+25604n-21912)B^6$$

$$\pm \frac{n^{2}B^{2}}{8} [16n^{2} - 48n + 41 - \frac{n^{4}}{8} (160n^{4} - 592n^{3} + 1316n^{2} - 2159n + 1578)B^{2} + \frac{n^{8}}{768} (24576n^{6} - 90784n^{5} + 312128n^{4} - 817204n^{3} + 1248835n^{2} - 1261972n + 736236)B^{4}]^{1/2}$$
(27)

where $\Delta E_{n_1n_2} = E + 1/2n^2$ is a Zeeman shift, and the indexes n_1 and n_2 denote the quantum numbers of the oscillator. The correspondences with a principal quantum number n and a quantum number k labeling the states inside a given diamagnetic multiplet are $n = |m| + n_1 + n_2 + 1$ and $k = n_2$. The form of the expansion for the pair of states (20) and (02) is slightly different because of their degeneracy (inside a subspace of given parity and m).

References

- Bender C M, Mlodinow L D and Papanicolaou N 1982 Phys. Rev. A 25 1305 - 1314
- Goodson D Z and Watson D K 1993 Phys. Rev. A 48 2668 2678
- Herzberg G 1945 Molecular Spectra and Molecular Structure. II.
 Infrared and Raman Spectra of Polyatomic Molecules
 (Princeton: D. Van Nostrand Company) Chapter II, 5c

Hulet R G and Kleppner D 1983 Phys. Rev. Lett. 51 1430 - 1433

- Germann T C, Herschbach D R, Dunn M and Watson D K 1995 Phys. Rev. Lett. **74** 658 - 661
- Kleppner D, Littman M G and Zimmerman L 1983 in *Rydberg States* of Atoms and Molecules, ed R F Stebbings and F B Dunning (Cambridge: Cambridge University) pp 73 - 116
- Liang J, Gross M, Goy P and Haroche S 1986 *Phys. Rev.* A **33** 4437 4439
- Turbiner A V 1984 J. Phys. A: Math. Gen. 17 859 875
- Vainberg V M, Popov V S and Sergeev A V 1990 *Sov. Phys. JETP* **71** 470 - 477
- Wunner G, Kost M and Ruder H 1986 Phys. Rev. A 33 1444 1447
- Zimmerman M L, Kash M M and Kleppner D 1980 *Phys. Rev. Lett.* **45** 1092 - 1094

Table 1. Branch points g_c for various pairs of states. Large-*m* approximations (22) and (23) for m = 100 are included in square brackets

	(10) - (02)		(11) - (03)		(10) - (04)	
т	Real	Imaginary	Real	Imaginary	Real	Imaginary
10	0.253 651	0.106 016	0.157 41	0.154 97	0.552	0.016
20	0.336 797	0.083 470	0.284 337	0.137 521	0.666 9	0.007 0
30	0.366 535	0.069 959	0.331 033	0.117 927	0.706 83	0.003 99
50	0.390 962	0.055 155	0.369 482	0.094 246	0.739 417	0.001 931
100	0.409 628 [0.428 57]	0.039 446 [0.039 83]	0.398 841 [0.428 6]	0.067 928 [0.069 0]	0.764 264	0.000 703

Figure captions

- Figure 1. The dependence of the scaled energy \tilde{E} on the coupling parameter g for n = |m|+1 states corresponding to the ground state of the oscillator ($n_1 = n_2 = 0$). Chain curve is the border of continuum spectrum corresponding to the lowest Landau level $(1+m^{-1})g^{1/2}$ shown for m=1.
- Figure 2. The vibrational energy of the even parity states (solid lines) and odd parity states (dashed lines) in the large *m* limit. The curves are labeled by harmonic oscillator quantum numbers n_1, n_2 .
- Figure 3. The vibrational energy levels in m = 30 azimuthal subspace obtained by summation of 1/m-expansion. The ionization threshold is shown by chain line.
- Figure 4. Similar to figure 3 but for m = 10 subspace. The results of the standard perturbation theory are shown by dotted lines.
- Figure 5. The curves of the constant ratio ω_1 / ω_2 on the scaled (*F*, *B*)plane where Fermi-like resonances occur in parallel electric and magnetic fields.



Fig. 2



Fig. 3









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