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 $n-|m|$.

Here, we pay attention to the level crossings in external fields. As a typical non-separable problem, we study in detail a hydrogen atom in a uniform magnetic field directed perpendicular to the plane of the circular orbit.

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 quasi-crossings are identified as Fermi resonances. The energies and complex branch points are calculated by the semiclassical method of $1/|m|$-expansion.

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

In cylindrical coordinates, the effective potential in the Schrödinger equation is:

$$V_{\text{eff}}(\rho,z) = \frac{m^2 - 1/4}{2\rho^2} - \frac{1}{r} + \frac{B^2}{8}\rho^2$$

Here, we use atomic units. The paramagnetic interaction $\frac{B}{2}L_z$ is an integral of motion equal $\frac{B}{2}m$, and it will be omitted further.

Let $m > 0$. A convenient way to exhibit explicitly the large-m limit is to define rescaled variables: $\rho = m^2\rho'$, $z = m^2 z'$, $E = m^{-2}E'$, $B = m^{-3}B'$ and assume that B' be m independent. Then we arrive to an equation with the effective potential

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

in which $1/m$ plays the role of the Planck's constant, or m^2 imitates the mass.

To solve this equation , 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 effective potential and describe a classical particle resting on the plane (ρ', z'), the energy being $E_0' = V'_{\text{eff}}(\rho'_0, z'_0)$. 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 $\dfrac{B'^2}{4} r_0'^4 + r_0' - 1 = 0$.

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

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

that leads to an equation with a new effective potential

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

where $g = B'^2 r_0'^4 / 4 = 1 - r_0'$ 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.

Since the equilibrium radius $\tilde{r}_0$ and the velocity $1 / \tilde{r}_0$ remain unity, the classical dynamics in a potential $\tilde{V}(\tilde{x},\tilde{y},\tilde{z}) = -\dfrac{1-g}{\tilde{r}} + \dfrac{g}{2}\tilde{\rho}^2$ 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.

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 $U(\xi,\eta)$:

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

where

$$U(\xi,\eta) = -[(1+g)\xi^3 + \frac{3}{2}(1-g)\xi\eta^2]m^{-1/2}$$

$$+\left[\left(\frac{3}{2}+g \right)\xi^4 - \frac{3}{8}(1-g)\eta^4 + 3(1-g)\xi^2\eta^2 - \frac{1}{8} \right]m^{-1} + \ldots,$$

$$\varepsilon = (\widetilde{E} - \widetilde{E}_0)m = (n_1 + 1/2)\omega_1 + (n_2 + 1/2)\omega_2$$

$$+ \text{(anharmonic terms)},$$

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

are the frequencies of normal oscillations. The anharmonic terms in the energy represent a series in powers of $1/m$ whose coefficients are calculated from the recurrence relations.

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 resulting curves $\widetilde{E}(g)$ are shown in the Figure 1. 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 $\widetilde{E}_0(g) = -\frac{1}{2} + \frac{3}{2}g$. The figure 1 gives a survey of the entire range of the field strengths from the zero field $\widetilde{E}(0) = -m^2/2(m + n_1 + n_2 + 1)^2$ up to the infinite field limit $\widetilde{E}(1) = (m + 2n_1 + 1)/m$.

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

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 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 CO_2 molecule.

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 are $H_{11} = \frac{3}{2}\omega_1 + \frac{1}{2}\omega_2$ and $H_{22} = \frac{1}{2}\omega_1 + \frac{5}{2}\omega_2$. The anharmonicity that mixes the oscillator's eigenstates is $u_{12}\xi\eta^2 m^{-1/2}$, where the potential constant is $u_{12} = 3(g-1)/2$. Solving the secular equation one obtains the energy

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

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 $g = 0$ corresponds 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.

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.

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 $g_c^{(n_1 n_2)-(n_1' n_2')} = (r^2 - 1) / (r^2 + 3)$.

For large but finite m, the levels of the same parity join in branch points whose imaginary part is small.

Let us consider (10) and (02) states. Using simple algebra, one can find

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

To obtain the exact values of g_c, we calculate the complex roots of the function $[\varepsilon_{n_1 n_2}(g) - \varepsilon_{n_1' n_2'}(g)]^2$ 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 are also given for comparison.

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

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

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.

able 1. Branch points g_c for various pairs of states.

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	(10) - (02)		(11) - (03)		(10) - (04)	
	Real	Imaginary	Real	Imaginary	Real	Imaginary
0	0.253 651	0.106 016	0.157 41	0.154 97	0.552	0.016
0	0.336 797	0.083 470	0.284 337	0.137 521	0.666 9	0.007 0
0	0.366 535	0.069 959	0.331 033	0.117 927	0.706 83	0.003 99
0	0.390 962	0.055 155	0.369 482	0.094 246	0.739 417	0.001 931
00	0.409 628	0.039 446	0.398 841	0.067 928	0.764 264	0.000 703
	[0.428 57]	[0.039 83]	[0.428 6]	[0.069 0]		

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.