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Effects of a Magnetic Field of the Arbitrary Strength on the Motion of a Rydberg Electron around a Polar Molecule

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ABSTRACT: In one of our previous papers we studied analytically the classical bound motion of a Rydberg electron around a polar molecule. In the present paper we study analytically how the classical bound motion in this system is affected by a magnetic field **B** along the electric dipole. We obtain analytical results for the arbitrary strength of the magnetic field. We show that the presence of the magnetic field opens up new ranges of the bound oscillatory-precessional motion of the Rydberg electron, the oscillations being in the meridional direction (θ-direction) and the precession being along parallels of latitude (φ-direction). In particular, it turns out that in one of the new rages of the motion, the period of the θ-oscillations has the non-monotonic dependence on primary parameter of the system. This is is a *counterintuitive results*.

Keywords: polar molecule; Rydberg electron; magnetic field; classical motion; periodic orbits Email: goks@physics.auburn.edu

1. INTRODUCTION

In the literature there were classical studies of the motion of an electron in the field of a point-like electric dipole. This is one of the most fundamental problems in atomic physics – next to hydrogen atoms. In 1968, Fox [1] provided the initial analytical description of this classical problem. He demonstrated that only for the zero total energy is it possible for the system to have bound motion and that this motion is confined to a sphere. He presented the final results only in terms of integrals (i.e., in the form of quadratures). Besides, he did not provide a qualitative description of the motion.

In 1995, Jones [2] studied a particular case of this classical problem limited to a semicircular orbit along a meridian on a sphere. In his description the moving particle was positively charged. So, he found that its motion is identical to the motion of a pendulum.

In 1996, McDonald [3] presented a classical study where he limited himself to two types of circular (or semicircular) orbits. One type of the orbit was actually the same as in paper [2]. Another type was a circular orbit perpendicular to the dipole moment, i.e., the orbit along a certain parallel of latitude. For the general case, he reproduced some analytical results from paper [1]. He also pointed out that the motion generally should consist of large oscillations with respect to the polar angle θ combined with a slow precession about the direction of the dipole moment.

In 2020 in paper [4] we presented a detailed classical analytical description of the oscillatory-precessional motion of the electron in this system. We showed that in the general case of the oscillatory-precessional motion of the electron, both the θ-oscillations (i.e., in the meridional direction) and the φ-precessions (i.e., along parallels of latitude) are characterized by the same time scale – contrary to the statement from work [3]. In the general case, we presented the time evolution of the dynamical variable θ, the period T_θ of the θ-oscillations, the dependence of φ on θ, and the change of the angular variable φ during one half-period of the θ-motion in the forms of one-fold integrals.

We complemented these results by the corresponding explicit analytical expressions for relatively small values of the projection p_φ of the angular momentum on the axis of symmetry. We also presented a general condition for the trajectory of the electron would become a closed curve. We listed examples of the values of p_φ for the closed curves to occur. For the case of the maximum possible value of p_φ, we produced an explicit analytical result for the period of the revolution of the electron along the parallel of latitude. Finally, for the case of the zero projection of the angular momentum on the dipole, we obtained an explicit analytical result for the dependence of the time t on θ.

In the present paper, we consider analytically a more complicated problem: namely, the situation where there is a uniform magnetic field parallel to the electric dipole. The magnetic field can be of the arbitrary strength. We show that the presence of the magnetic field opens up new ranges of the bound oscillatory-precessional motion of the Rydberg electron.

2. CLASSICAL BOUND ORBITS

Following papers [1, 4], we consider an electric dipole, having the dipole moment D, centered at the origin. The motion of an electron in the field of the dipole is analyzed in spherical polar coordinates (r, θ, φ) with the z-axis chosen along the dipole axis, such that the positive pole points to the upper hemisphere. The system is under a uniform magnetic field **B** along the z-axis.

The Lagrangian has the form

$$L = m[(dr/dt)^2 + r^2(d\theta/dt)^2 + r^2\sin^2\theta\,(d\varphi/dt)^2]/2 + eD\cos\theta/r^2 - (mr^2/2)(d\varphi/dt)\Omega, \tag{1}$$

where m and e are the mass and the absolute value of the electron charge, respectively. The quantity Ω in Eq. (1) is the magnetic field scaled to the dimension of frequency:

$$\Omega = eB/(mc). \tag{2}$$

It should be emphasized that if **B** is parallel to the electric dipole, then $\Omega > 0$, while if **B** is antiparallel to the electric dipole, then $\Omega < 0$.

From one of the Lagrange equations of the motion

$$d[\partial L/\partial(d\varphi/dt)]/dt = \partial L/\partial\varphi = 0 \tag{3}$$

follows that

$$\partial L/\partial(d\varphi/dt) = mr^2\,[(d\varphi/dt)\sin^2\theta - \Omega/2] = p_\varphi = \text{const.} \tag{4}$$

Physically, p_φ is the projection of the angular momentum (generalized for the presence of the magnetic field) on the axis of the electric dipole.

From Eq. (4) we find

$$d\varphi/dt = [\Omega/2 + p_\varphi/(mr^2)]/\sin^2\theta, \tag{5}$$

so that

$$\varphi(t) = \int dt\,\{\Omega/2 + p_\varphi/[mr^2(t)]\}/\sin^2\theta(t). \tag{6}$$

Equation (6) allows to determine the time evolution of the φ-coordinate if the time-evolution of r- and θ-coordinates are known.

From the other Lagrange equations of the motion

$$d[\partial L/\partial(dr/dt)]/dt = \partial L/\partial r \tag{7}$$

we find:

$$m(d^2r/dt^2) – [mr(d\theta/dt)^2 + mr\sin^2\theta\ (d\varphi/dt)^2 – 2eD\cos\theta/r^3 + mr\Omega(d\varphi/dt)/2. \quad (8)$$

From the Lagrangian in Eq. (1) follows the expression for the total energy E:

$$E = m[(dr/dt)^2 + r^2(d\theta/dt)^2 + r^2\sin^2\theta\ (d\varphi/dt)^2]/2 – eD\cos\theta/r^2 + (mr^2/2)(d\varphi/dt)\Omega. \quad (9)$$

Now we multiply both sides of Eq. (8) by r and add to it Eq. (9) multiplied by 2 to obtain the equation containing only the variable r (the angular variables got separated):

$$2E = mr(d^2r/dt^2) + m(dr/dt)^2 = md[r(dr/dt)]/dt. \quad (10)$$

By integrating Eq. (10), we get

$$r(dr/dt) = 2Et/m + \text{const}. \quad (11)$$

From Eq. (11) we draw the following important conclusions. If $E > 0$, then in the course of time one would have $dr/dt > 0$, so that the electron moves away from the dipole. If $E < 0$, then in the course of time one would have $dr/dt < 0$, so that the electron would collapse to the dipole. Thus, the only possibility for the bound motion is for $E = 0$ and const = 0 in Eq. (110. In this case one has $dr/dt =0$, so that the bound motion occurs on a sphere of a fixed radius r and the dynamical variables are only θ and φ.

For $E = 0$ and r = const, Eq. (9) becomes:

$$m[(dr/dt)^2 + r^2(d\theta/dt)^2 + r^2\sin^2\theta\ (d\varphi/dt)^2]/2 – eD\cos\theta/r^2 + (mr^2/2)(d\varphi/dt)\Omega = 0. \quad (12)$$

On substituting $d\varphi/dt$ from Eq. (5) in Eq. (12), we obtain:

$$(d\theta/dt)^2 + p_\varphi^2/(m^2r^4\sin^2\theta) + 2\ p_\varphi\Omega/(mr^2\sin^2\theta) + 3\Omega^2/(4\sin^2\theta) – 2eD\cos\theta/(mr^4) = 0. \quad (13)$$

Thus, we separated the θ-motion from the φ-motion.

We denote $x = \cos\theta$. In terms of the variable x, Eq. (13) can be represented in the form

$$(dx/dt)^2 = [2eD/(mr^4)]\ y(x, K), \qquad y(x, K) = (–x^3 + x – K), \quad (14)$$

where

$$K = [3mr^4/(8eD)][\Omega + 2p_\varphi/(mr^2)][\Omega + 2p_\varphi/(3mr^2)]. \quad (15)$$

Equation (14) is mathematically identical to Eq. (3) from paper [4]. The difference is only in the definition of the quantity K.

The cubic equation $–x^3 + x – K = 0$ has the following tree roots:

$$x_1(K) = \{–(–2)^{1/3} + [(–2)^{2/3}/6][(729K^2 – 108)^{1/2} – 27K]^{2/3}\}/[(729K^2 – 108)^{1/2} – 27K]^{1/3}, \quad (16)$$

$$x_2(K) = (–1)^{2/3}2^{1/3}/[(729K^2 – 108)^{1/2} – 27K]^{1/3} – (–1)^{1/3}[(729K^2 – 108)^{1/2} – 27K]^{1/3}/(2^{1/3}3), \quad (17)$$

$$x_3(K) = 2^{1/3}/[(729K^2 – 108)^{1/2} – 27K]^{1/3} – [(729K^2 – 108)^{1/2} – 27K]^{1/3}/(2^{1/3}3). \quad (18)$$

Figure 1 shows a plot of all three roots $x_1(K)$, $x_2(K)$ and $x_3(K)$. Namely, the branch that starts at (0, –1) and ends at $(–2/3^{3/2}, –1/3^{1/2})$ is $x_1(K)$. The branch that starts at $(–2/3^{3/2}, –1/3^{1/2})$ and ends at $(2/3^{3/2}, 1/3^{1/2})$ is $x_2(K)$. The branch that starts at $(2/3^{3/2}, 1/3^{1/2})$ and ends at (0, 1) is $x_3(K)$.

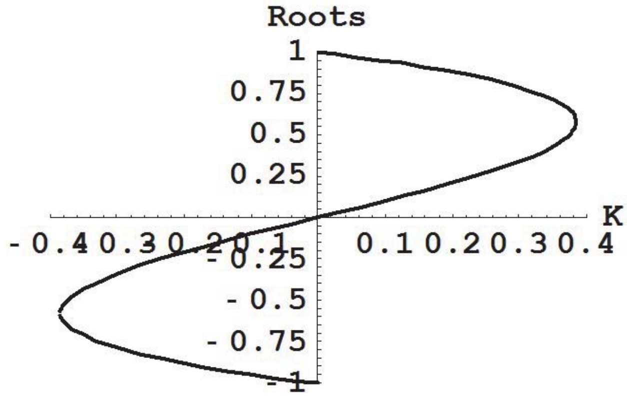

Fig. 1. Plot of all three roots $x_1(K)$, $x_2(K)$ and $x_3(K)$ of the polynomial $y(x, K) = (-x^3 + x - K)$ from Eq. (14). Namely, the branch that starts at (0, –1) and ends at $(-2/3^{3/2}, -1/3^{1/2})$ is $x_1(K)$. The branch that starts at $(-2/3^{3/2}, -1/3^{1/2})$ and ends at $(2/3^{3/2}, 1/3^{1/2})$ is $x_2(K)$. The branch that starts at $(2/3^{3/2}, 1/3^{1/2})$ and ends at (0, 1) is $x_3(K)$.

Since $(dx/dt)^2$ in the left side of Eq. (14) cannot be negative, then for the θ-motion to be possible, the polynomial $y(x, K) = (-x^3 + x - K)$ in Eq. (14) should be non-negative. Let us study this in detail.

We denote

$$u = mr^4\Omega/p_\varphi, \tag{19}$$

assuming that p_φ is not zero. (In the case of $p_\varphi = 0$, Eq. (15) yields the value $K = 3mr^4\Omega^2/(8eD)$ that cannot be negative.) So, $u > 0$ if the the magnetic field is parallel to the projection of the angular momentum on the dipole or $u < 0$ if the magnetic field is antiparallel to the projection of the angular momentum on the dipole. Then Eq. (15) takes the form:

$$K = [p_\varphi/(2meD)](3u^2/4 + 2u + 1). \tag{20}$$

A simple analysis of the quadratic trinomial in the right side of Eq. (20) demonstrates that for $-2 < u < -2/3$ (which is possible if the magnetic field is antiparallel to the projection of the angular momentum on the dipole), the quantity K in Eq. (14) is negative. This opens up additional ranges of the θ-motion compared to the absence of the magnetic field, as presented below.

Figure 2 shows the plot of the function y(x, K) from Eq. (14) versus x for the following 6 values of the quantity K (from the bottom curve to the top curve): $2/3^{3/2}$, 0.2, 0, –0.2, $-2/3^{3/2}$, –0.7, –1.

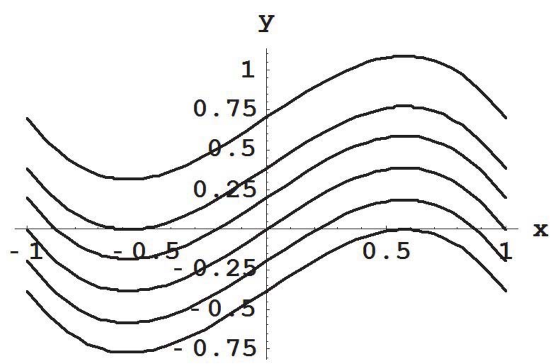

Fig. 2. Plot of the function y(x, K) from Eq. (14) versus x for the following 6 values of the quantity K (from the bottom curve to the top curve): $2/3^{3/2}$, 0.2, 0, –0.2, $-2/3^{3/2}$, –0.7, –1.

The following can be seen from Fig. 2, as well as from the above analytical results.

A. For $0 < K < 2/3^{3/2}$, the range of the θ-motion is between $x_2(K)$ and $x_3(K)$.

B. For $-2/3^{3/2} < K < 0$, the range of the θ-motion is between $x_2(K)$ and 1, as well as between –1 and $x_1(K)$, the latter range being near the South pole of the sphere, to which the bound motion is confined. We note that $-1 < x_1(K) < 1/3^{1/2}$.

C. For $K < -2/3^{3/2}$, the θ-motion is allowed in the entire range $-1 < x < 1$.

Thus, the magnetic field **B** opens up new ranges of the θ-motion – compared to the B = 0 case where the possible values of K were only $0 < K < 2/3^{3/2}$ and the range of the θ-motion was only between $x_2(K)$ and $x_3(K)$.

Now we study limiting cases.

1. The particular case of $K = K_{max} = 2/3^{3/2}$. There is no θ-motion, just as the B = 0 situation. The electron moves in a circular path along the parallel of latitude corresponding to $\cos\theta = 1/3^{1/2}$, i.e., θ = 0.9553 rad = 54.74 degrees. From Eq. (5) it follows that the electron rotates with the constant angular velocity

$$d\varphi/dt = (3/4)[\Omega + 2p_\varphi/(mr^2)], \tag{21}$$

corresponding to the period

$$T = (8\pi/3)/[\Omega + 2p_\varphi/(mr^2)]. \tag{22}$$

For $K = 2/3^{3/2}$, Eq. (15) can be rewritten as follows:

$$[\Omega + 2p_\varphi/(mr^2)]\,[\Omega + 2p_\varphi/(3mr^2)] = 16eD/(3^{5/2}mr^4). \tag{23}$$

Using Eq. (23), we can represent the period from Eq. (22) in the alternative form:

$$T = [3^{3/2}\pi mr^4/(2eD)\,[\Omega + 2p_\varphi/(3mr^2)]. \tag{24}$$

From Eq. (23) it is seen that neither $[\Omega + 2p_\varphi/(mr^2)]$ nor $[\Omega + 2p_\varphi/(3mr^2)]$ can be equal to zero. So, Eq. (22) for the period cannot yield infinity and Eq. (24) for the period cannot yield zero.

We introduce the following notations:

$$w = p_\varphi/(meD)^{1/2}, \qquad b = 3mr^2\Omega/(meD)^{1/2}. \tag{25}$$

Physically, w is the scaled dimensionless projection of the angular momentum on the dipole and b is the scaled dimensionless magnetic field. In the notations from Eq. (25), we rewrite Eq. (23) as follows:

$$b^2 + 8wb + 12\,w^2 - 16/3^{1/2} = 0. \tag{26}$$

Equation (26) has the following two solutions:

$$b_\pm = -4w \pm (4w^2 + 16/3^{1/2})^{1/2}. \tag{27}$$

Figure 3 shows the dependence of the scaled magnetic field b on the scaled projection of the angular momentum w for both solutions. The upper and lower curves correspond to b_+ and b_-, respectively.

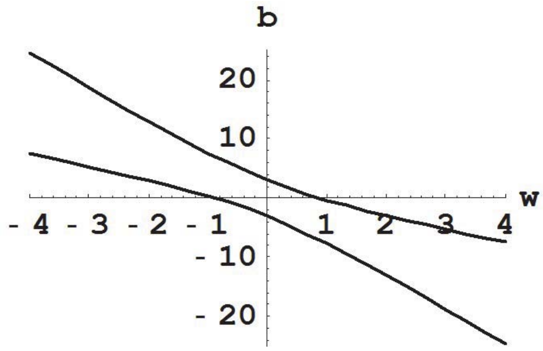

Fig. 3. Dependence of the scaled magnetic field $b = 3mr^2\Omega/(meD)^{1/2}$ on the scaled projection of the angular momentum $w = p_\varphi/(meD)^{1/2}$ for both solutions of Eq. (26). The upper and lower curves correspond to b_+ and b_-, respectively.

It is seen that for any value of the projection of the angular momentum, there are two values of the magnetic field enabling the uniform circular motion along the parallel of latitude at $\cos\theta = 1/3^{1/2}$. In comparison, for B = 0 case, such motion was possible for only two particular values of the projection of the angular momentum corresponding to $w = \pm 2/3^{3/4} = \pm 0.8774$.

Another interesting point: the presence of the magnetic field makes this kind of motion possible even for the zero projection of the angular momentum – provided that the scaled magnetic field is either $b = 4/3^{1/4} = 3.039$ or $b = -4/3^{1/4} = -3.039$. We remind that negative values of the magnetic field and of the projection of the angular momentum mean that they are antiparallel to the electric dipole.

2. The particular case of K = 0. From Eq. (15) is follows that K = 0 for the following two values of the scaled (to the frequency dimension) magnetic field:

$$\Omega_1 = -2p_\varphi/(mr^2), \qquad \Omega_2 = -2p_\varphi/(3mr^2). \tag{28}$$

The subcase of $\Omega = \Omega_2$ does not differ from the general case of the oscillatory θ-motion between θ = 0 and θ = π/2 simultaneously with the precessional φ-motion. The subcase of $\Omega = \Omega_1$ is more interesting, as presented below.

When $\Omega = \Omega_1$, from Eq. (5) it follows that φ = const, i.e., there is no φ-motion. The electron oscillates along a semicircle located in a meridional plane in the Northern hemisphere. At the absence of the magnetic field **B** this kind of motion was possible only for $p_\varphi = 0$. Thus, the magnetic field enables this motion for any projection p_φ of the angular momentum – under the condition $\Omega = -2p_\varphi/(mr^2)$.

As presented in our previous paper [4], after introducing a scaled dimensionless time

$$\tau = t[2eD/(mr^4)]^{1/2}, \tag{29}$$

Eq. (14) can be rewritten in the form:

$$d\tau = \pm dx/(-x^3 + x - K)^{1/2}. \tag{30}$$

As noted in paper [4], for K = 0, Eq. (30) can be integrated analytically to yield the following explicit dependence of the scaled time τ on x, i.e., the dependence of τ on cosθ:

$$\tau(x) = -\{\pm 2i\,\mathbf{F}[\arcsin(-x)^{1/2}, -1]\}, \tag{31}$$

where $\mathbf{F}(\alpha, q)$ is the incomplete elliptic integral of the first kind. For the range $0 < x < 1$ where the motion occurs, the right side of Eq. (31) is actually real despite the formal appearance of the imaginary unit i. In particular, for $x \ll 1$, the following explicit result was obtained from Eq. (31) in paper [4]:

$$x \approx \pm\tau/2. \tag{32}$$

Figure 4 (adopted from Fig. 3 from paper [4]) shows the temporal and spatial evolution of the electron for one half-cycle of the θ-oscillations for the case of K = 0. The full period of oscillations is as follows (in terms of the scaled time):

$$\tau_0 = 4\tau(1) = 8\pi^{1/2}\Gamma(5/4)/\Gamma(3/4) = 10.488, \quad (33)$$

where Γ(s) is the gamma-function. In the usual units this corresponds to the period

$$T = 10.488\ [mr^4/(2eD)]^{1/2}. \quad (34)$$

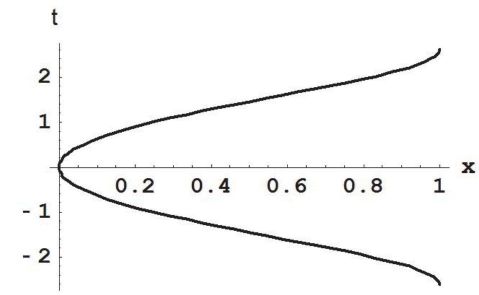

Fig. 4. Dependence of the scaled time τ (defined in Eq. (29)) on x = cosθ during one half-period of the electron oscillation along a semicircular path through the north pole of the upper hemisphere for K = 0. (Adopted from Fig. 3 of paper [4].)

Now we proceed to the general case of an arbitrary K. Based on Eq. (13), the dependence of the scaled time τ on x (i.e., the dependence of τ on cosθ) in the general case has the form:

$$\tau(x, K) = \pm \int_{x_{min}(K)}^{x} dz/(-z^3 + z - K)^{1/2}. \quad (35)$$

The inter-dependence of the angular variable φ and the angular variable x = cosθ is given as follows (according to paper [4]):

$$\varphi(K, x) = |K|^{1/2} \int_{x_{min}(K)}^{x} dz/[(1 - z^2)[(-z^3 + z - K)^{1/2}]. \quad (36)$$

In Eqs. (35), (36), the lower limit of the integration is the smaller of the turning points for the corresponding range of the θ-motion.

The scaled period T_θ of the θ-motion is given by the following formula (in units of $mr^4/(2eD)$):

$$T_\theta(K) = 2 \int_{x_{min}(K)}^{x_{max}(K)} dz/(-z^3 + z - K)^{1/2}. \quad (37)$$

The upper limit of the integration in Eq. (37) depends on which range of K (out of the ranges A, B, and C specified above) we consider.

For $0 < K < K_{max}=2/3^{3/2}$ (the range A), both the θ- and φ-motions were studied analytically and illustrated pictorially in paper [4]. Here for completeness of the presentation we reproduce the dependence of the period T_θ on K for this range – see Fig. 5 adopted from Fig. 6 of paper [4]. In this range of K, the limits of the integration in Eq. (37) are $x_{min}(K) = x_2(K)$, $x_{max}(K) = x_3(K)$.

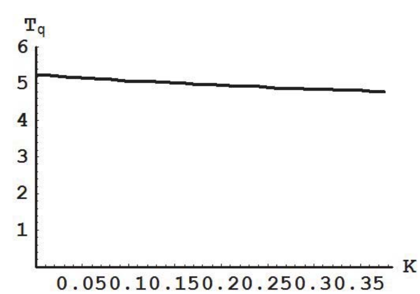

Fig. 5. Dependence of the scaled period $T_è$ of the è-motion on the parameter K (defined by Eq. (15)) for the range of $0 < K < K_{max}=2/3^{3/2}$ [4]. The period $T_è$ is in units of $mr^4/(2eD)$.

For $-2/3^{3/2} < K < 0$ (the range B), there are two possible ranges of the θ-motion (see Fig. 2):

B.1) $x_2(K) < x < 1$; B.2) $-1 < x < x_1(K)$. For the case B.1, the limits of the integration in Eq. (37) are $x_{min}(K) = x_2(K)$, $x_{max}(K) = 1$. Figure 6 presents the dependence of the period T_θ on K for the case B.1.

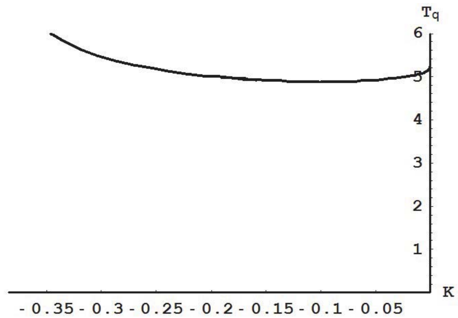

Fig. 6. Dependence of the scaled period T_θ of the θ-motion on the parameter K (defined by Eq. (15)) for the range $-2/3^{3/2} < K < 0$ and the range of the è-motion $x_2(K) < x < 1$ (case B.1). The period T_θ is in units of $mr^4/(2eD)$.

It is seen that in this range (which became possible due to the magnetic field), the period T_θ has the non-monotonic dependence on K – in distinction to the range $0 < K < 2/3^{3/2}$. As |K| increases from zero, the period T_θ first decreases, then reaches a minimum, and then increases. The non-monotonic dependence of the period T_θ of the θ-motion on parameter K is a *counterintuitive result*.

For the case B.2 (also made possible due to the magnetic field) the limits of the integration in Eq. (37) are $x_{min}(K) = -1$, $x_{max}(K) = x_1(K)$. Figure 7 presents the dependence of the period T_θ on K for this case. In particular, it is seen that $T_\theta = 0$ for $K = 0$. Physically, this corresponds to the fact that for K = 0, there is no interval for the θ-motion in the Southern hemisphere.

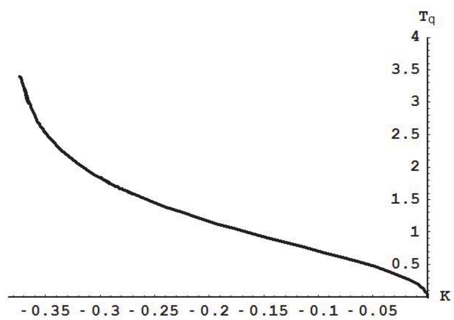

Fig. 7. Dependence of the scaled period T_θ of the θ-motion on the parameter K (defined by Eq. (15)) for the range $-2/3^{3/2} < K < 0$ and the range of the θ-motion $-1 < x < x_1(K)$ (case B.2). The period T_θ is in units of $mr^4/(2eD)$.

Finally we consider the situation where $K < -2/3^{3/2}$ (the range C). In this situation, the limits of the integration in Eq. (37) are –1 and 1. Figure 8 presents the dependence of the period T_θ on K for this range of K.

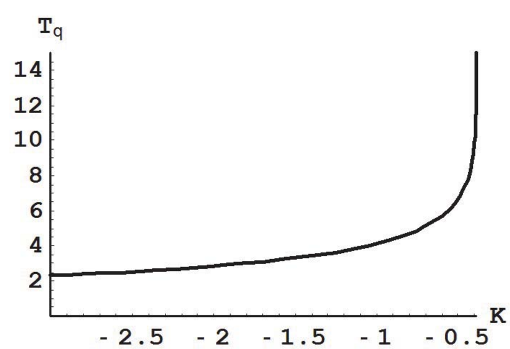

Fig. 8. Dependence of the scaled period T_θ of the θ-motion on the parameter K (defined by Eq. (15)) for the range $K < -2/3^{3/2}$ (range C). The period T_θ is in units of $mr^4/(2eD)$.

3. CONCLUSIONS

We studied how the classical bound motion of a Rydberg electron around a polar molecule is affected by a magnetic field along the electric dipole. We obtained analytical results for the arbitrary strength of the magnetic field.

We showed that the presence of the magnetic field opens up new ranges of the bound oscillatory-precessional motion of the Rydberg electron, the oscillations being in the meridional direction (è-direction) and the precession being along parallels of latitude (ö-direction).The following results should be especially emphasized.

1. As the magnetic field opened up several new ranges of the parameter K (defined by Eq. (15)), it turned out that in one of these ranges – namely, on the range $0 < K < 2/3^{3/2}$ – the period of the θ-oscillations has the non-monotonic dependence on K. This is a *counterintuitive results*.
2. For the particular case where the Rydberg electron oscillates along a semicircle located in a meridional plane in the Northern hemisphere: at the absence of the magnetic field **B** this kind of motion was possible only for the zero projection of the angular momentum p_φ on the electric dipole. In distinction, the magnetic field enables this motion for any value of p_φ – under the condition $\Omega = -2p_\varphi/(mr^2)$, where $\Omega = eB/(mc)$ is the magnetic field scaled to the units of frequency.
3. For the particular case where the Rydberg electron executes the uniform circular motion along the parallel of latitude at $\cos\theta = 1/3^{1/2}$: a proper choice of the magnetic field (given by Eq. (27) and illustrated by Fig. 3) makes this motion possible for any value of the projection p_φ of the angular momentum on the dipole. In comparison, at the absence of the magnetic field, such motion was possible for only two particular values of the projection of the angular momentum corresponding to $p_\varphi/(meD)^{1/2} = \pm 2/3^{3/4} = \pm 0.8774$.

We believe that our classical results provide a physical insight in the complicated dynamics of a Rydberg electron around a polar molecule for an arbitrary strength of the magnetic field.

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