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Non-Lie Top Tunneling and Quantum Bilocalization in Planar Penning Trap*

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Abstract—We describe how a top-like quantum Hamiltonian over a non-Lie algebra appears in the model of the planar Penning trap under the breaking of its axial symmetry (inclination of the magnetic field) and tuning parameters (electric voltage, magnetic field strength and inclination angle) at double resonance. For eigenvalues of the quantum non-Lie top, under a specific variation of the voltage on the trap electrode, there exists an avoided crossing effect and a corresponding effect of bilocalization of quantum states on pairs of closed trajectories belonging to common energy levels. This quantum tunneling happens on the symplectic leaves of the symmetry algebra, and hence it generates a tunneling of quantum states of the electron between the 3D-tori in the whole 6D-phase space. We present a geometric formula for the leading term of asymptotics of the tunnel energy-splitting in terms of symplectic area of membranes bounded by invariantly defined instantons.

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1. INTRODUCTION

The ideal Penning trap is created by a homogeneous magnetic field and by a quadratic electric potential with a saddle profile in 3D-space. Its Hamiltonian is just a hyperbolic-type harmonic oscillator with three frequencies. Such devices are used for long time confinement of individual charges [1]–[3]. Of course, the Hamiltonians of real traps contain not only the harmonic part, but also some anharmonic potentials. In this work, we deal with a planar trap with ring electrodes, as in [4]–[6], creating, in addition to quadratic, also cubic, quartic, etc. terms in the electric potential near the trap center.

We study the main hyperbolic $2:(-1):2$ resonance of the trap frequencies suggested in [7]. We also break the usual axial symmetry and assume that the magnetic field deviates by a small angle ε from the saddle axis of the trap. We specially choose the deviation angle to obtain the secondary $4:(-2):1$ resonance in the ε-perturbing part of the Hamiltonian, as in [7]–[9].

In such a double-resonance trap, the cubic and quartic terms of the electric potential generate a top-like Hamiltonian over a non-Lie analog of the $su(1,1)$ algebra [9]. This non-Lie algebra consists of bisymmetries (integrals of motion) of the quadratic part of the trap Hamiltonian. The dynamics of the non-Lie top is the dynamics of symmetries under an anharmonic perturbation. This dynamics determines the whole evolution of the charge in the trap.

In particular, the equilibrium points of the top dynamics (studied in [9], [10]) correspond to almost invariant 2D-tori in the original 6D-phase space of the system. Near the stable equilibrium points, the top Hamiltonian has families of closed trajectories fibrating the symplectic leaves of the bisymmetry

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algebra. Each of these closed trajectories corresponds to an almost invariant Liouville 3D-torus in the original phase space.

By an additional small variation of the voltage on the ring electrode of the trap, one can also obtain unstable equilibrium points of the top dynamics as well as separatrices on the symplectic leaves. In this case, some energy levels of the top Hamiltonian consist of pairs of closed curves. In the original phase space, each such a pair of curves corresponds to a pair of 3D-tori belonging to the same energy level of the moving charge. These pairs of Liouville 3D-tori are candidates for the tunneling of the charge in the framework of quantum mechanics.

Of course, the quantum treatment is not actual for macrotraps and even for microtraps whose frequencies are not in resonance or the resonance is degenerate (parabolic, like $1:0:0$). A discussion on the quantum behavior of planar Penning traps can be found, for instance, in [10], [11]. The general conclusion is the following: under the breaking of the axial symmetry and the tuning parameters at biresonance, the electron in the microtrap has to be treated as a quantum particle, since its discrete energy levels become "visible" and one cannot ignore its quantum properties.

For instance, a quantum tunneling of the electron from a 3D-torus to another one located near the same energy level can appear. Here we use the words "near the same," since there is actually some splitting or a gap between the energy levels of the electron states on the pair of tunneling related tori.

In the present paper, we consider a top-like quantum Hamiltonian over the non-Lie algebra appearing in the double-resonance Penning trap [7]–[9]. For this system one can prove the appearance of the avoided crossing effect and the bilocalization of quantum states on pairs of closed curves under specific tuning of the parameter of the top (by methods similar to [12], [13]).

The presence of controlling parameters is the key condition for the tunneling effects in systems with broken symmetry. In our model, such a parameter is just a small variation of the voltage on the trap electrode [11].

Note that the tunneling between closed curves on symplectic leaves of the symmetry algebra generates tunneling of quantum states of the electron between 3D-tori in the phase space of the trap.

In addition to the fact of bilocalization of eigenstates on two disconnected tori, it is important to known the gap between the energy levels split by the tunneling. We present a formula for the leading term of the exponential asymptotics of this energy splitting.

The obtained asymptotics for the tunnel splitting allows us to estimate the time of tunnel transitions of the electron states from one 3D-torus onto another. In the case of a microtrap, this time can be on the scale of microseconds [11]. Thus, tunneling can play a significant role in the dynamics of the electron in the Penning microtrap.

2. RESONANCE PENNING TRAP WITH BREAKING OF COMMUTATIVE SYMMETRY

In the planar Penning trap model under study, the electric field is created by three concentric electrodes lying in the same plane, namely, a circle of radius ρ_1 where the zero potential is maintained, a ring (annulus) with two radii $\rho_1 < \rho_2$ to which a constant potential W is applied, and the exterior of the ring where the zero potential is maintained. By (q_1, q_2) we denote the coordinates in this plane with origin at the center of the circular electrode, $r \stackrel{\text{def}}{=} \sqrt{q_1^2 + q_2^2}$, and by q_3 we denote the coordinate in the direction perpendicular to the plane. Let us introduce the dimensionless coordinates as follows: $x \stackrel{\text{def}}{=} q_1/\rho_1$, $y \stackrel{\text{def}}{=} q_2/\rho_1$, $\rho \stackrel{\text{def}}{=} r/\rho_1$, $z \stackrel{\text{def}}{=} q_3/\rho_1$. We consider the case where the outer radius of the ring electrode is much greater than the inner radius

$$\delta \stackrel{\text{def}}{=} \frac{\rho_1}{\rho_2} \ll 1.$$

In the half-space $q_3 \geq 0$, the potential V created by the electrodes has a stationary point with coordinate

$$q_3^0 = \rho_1 z^0, \qquad \text{where} \quad z^0 = \delta^{-1/3}\left(1 - \frac{1}{2}\delta^{2/3} + O(\delta^{4/3})\right).$$

Near this point, the potential energy (with regard to the fact that the electron charge is negative) can be represented as

$$-eV = eV_o \cdot u, \qquad u = \text{const} + \frac{\omega_0^2}{2}u^{[2]} + \beta u^{[3]} + \gamma u^{[4]} + \dots, \tag{1}$$

where V_0 is a certain voltage calibration, which we fix below, and $u^{[j]}$ are homogeneous polynomials of degree j in the coordinates ρ and z:

$$u^{[2]} = (z-z^0)^2 - \frac{1}{2}\rho^2, \qquad u^{[3]} = (z-z^0)\Big[(z-z^0)^2 - \frac{3}{2}\rho^2\Big],$$
$$u^{[4]} = (z-z^0)^4 - 3(z-z^0)^2\rho^2 + \frac{3}{8}\rho^4.$$

The formulas for the coefficients have the form (for details, see [6])

$$\omega_0^2 = 3\frac{W}{V_0}\delta^{4/3}\Big(1 - \frac{1}{2}\delta^{2/3} + O(\delta^{4/3})\Big), \quad \beta = -2\frac{W}{V_0}\delta^{5/3}(1 + O(\delta^{2/3})),$$
$$\gamma = \frac{5}{2}\frac{W}{V_0}\delta^2(1 + O(\delta^{2/3})).$$

In addition to the electric potential, the trap also contains a homogeneous magnetic field $\mathcal{B}$ deviated by a small angle ε from the axis (i.e., from the perpendicular to the plane of electrodes). We assume that the magnetic field is directed away from the stationary point of the electric potential towards the plane of electrodes.

Now we introduce a voltage calibration which is determined by the energy density of the magnetic field confining a charged particle inside the trap, $V_0 = e|\mathcal{B}|^2\rho_1^2/mc^2$. Here m and e are the mass and the value of the particle (electron) charge, and c is the speed of light. We also introduce the magnetic length $\rho_0 = \sqrt{\hbar c/e|\mathcal{B}|}$ and the effective Planck constant $h = \big(\rho_0/\rho_1\big)^2$.

In the energy units eV_0, the total Hamiltonian of the trap becomes

$$\hat{H} = (-ih\nabla - \mathcal{A})/2 + u. \tag{2}$$

Here $\mathcal{A}$ is the effective magnetic potential related to the magnetic field as $(\nabla \times \mathcal{A}) = \mathcal{B}/|\mathcal{B}|$, and the operation $\nabla = (\nabla_x, \nabla_y, \nabla_z)$ is taken in dimensionless coordinates (x, y, z).

The effective (dimensionless) magnetic field is defined by the unit vector $\mathcal{B}/|\mathcal{B}|$ which has three components $\mathcal{B}/|\mathcal{B}| = (\sin\varepsilon, 0, \cos\varepsilon)$ (assuming that x is the coordinate axis directed along the magnetic field projection on the plane of electrodes). Neglecting terms very small in ε, we represent the magnetic field as $\mathcal{B}/|\mathcal{B}| = b + \varepsilon\tilde{b} + O(\varepsilon^3)$, where $b = (0, 0, \omega)$, $\tilde{b} = (1, 0, 1/4)$, and $\omega = 1 - \varepsilon/4 - \varepsilon^2/2$. Thus, the effective magnetic field is given by the "principal part" b directed along the trap axis and by a small perturbation $\varepsilon\tilde{b}$ whose axial and longitudinal components relate as $1:4$. This is a specially chosen breaking of the commutative axial symmetry of the trap.

The quantity ω is the frequency of rotation in the longitudinal (x, y)-plane. Also, the quadratic part of the potential u contains the frequency ω_0 of oscillations in the direction of the z-axis. As is known [1], the relation $\omega > \sqrt{2}\omega_0$ guarantees the trapping regime (the boundedness of the particle trajectories). We subject the frequencies to a stronger resonance condition $\omega = \frac{3}{2}\omega_0$, which ensures that the trajectories are not only bounded but also periodic. In view of the above explicit formulas for the frequencies ω and ω_0, the resonance condition reads

$$\frac{4}{9}\Big(1 - \frac{\varepsilon}{4} - \frac{\varepsilon^2}{2}\Big)^2 = 3\frac{W}{V_0}\delta^{4/3}\Big(1 - \frac{1}{2}\delta^{2/3} + O(\delta^{4/3})\Big).$$

We assume that the geometric parameters of the trap are consistent with each other in scale as follows:

$$\delta^{1/3} = k\varepsilon, \qquad k \sim 1. \tag{3}$$

In this case, the above resonance condition can be represented up to $O(\varepsilon^2)$ as

$$\frac{W}{V_0} = \frac{4}{27\delta^{4/3}}\Big(1 - \frac{1}{2}\varepsilon + \frac{1}{2}\Big(\delta^{2/3} - \frac{15}{8}\varepsilon^2\Big)\Big). \tag{4}$$

This formula of *combined resonance* relates the potential W of the ring electrode of the trap, the value of the magnetic field (determining the voltage V_0), the angle ε of the magnetic field deviation from the trap axis, and the ratio of the ring electrode radii $\delta = \rho_1/\rho_2$.

From the above computations, we obtain the following statement.

Lemma 1. *Under the condition of combined resonance* (4)*, the coefficients of expansion* (1) *are given by the formulas*

$$\omega_0 = \frac{2}{3}\Big(1 - \frac{\varepsilon}{4} - \frac{\varepsilon^2}{2}\Big), \qquad \beta = -\frac{8k}{27} + O(\varepsilon), \qquad \gamma = \frac{10k^2}{27}. \tag{5}$$

The effective Hamiltonian describing the electron motion in a planar quantum Penning trap can be written as $\hat{H} = \hat{H}_0 + \varepsilon\hat{H}_1 + \varepsilon^2\hat{H}_2 + O(\varepsilon^3)$*, where*

$$\begin{aligned}
\hat{H}_0 &= \frac{1}{2}\Big[\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 - \frac{3}{2}\omega_0(x\hat{p}_y - y\hat{p}_x) + \omega_0^2(z - z^0)^2 + \frac{1}{16}\omega_0^2(x^2 + y^2)\Big],\\
\hat{H}_1 &= \frac{1}{8}\Big[y\hat{p}_x + (4(z - z^0) - x)\hat{p}_y - 4y\hat{p}_z - 3\omega_0(z - z^0)x + \frac{3}{4}\omega_0(x^2 + y^2)\Big]\\
&\quad + \beta(z - z^0)\Big[(z - z^0)^2 - \frac{3}{2}(x^2 + y^2)\Big],\\
\hat{H}_2 &= \frac{1}{128}\big[17y^2 + (x - 4(z - z^0))^2\big] + \gamma\Big[(z - z^0)^4 - 3(z - z^0)^2(x^2 + y^2) + \frac{3}{8}(x^2 + y^2)^2\Big],
\end{aligned}$$

and the quantum momentum is defined as $\hat{p} = -ih\nabla$.

After the change of variables

$$\begin{aligned}
&x = \sqrt{\frac{2}{\omega_0}}(x_+ + x_-), \qquad \hat{p}_x = \frac{1}{2}\sqrt{\frac{\omega_0}{2}}(\hat{p}_+ + \hat{p}_-), \qquad y = \sqrt{\frac{2}{\omega_0}}(\hat{p}_+ - \hat{p}_-),\\
&\hat{p}_y = -\frac{1}{2}\sqrt{\frac{\omega_0}{2}}(x_+ - x_-), \qquad z = \frac{x_0}{\sqrt{\omega_0}} + z^0, \qquad \hat{p}_z = \sqrt{\omega_0}\hat{p}_0
\end{aligned}$$

the principal part $\hat{H}_0$ *of this Hamiltonian has the normal form*

$$\hat{H}_0 = \frac{1}{4}\omega_0\big(2(\hat{p}_+^2 + x_+^2) - (\hat{p}_-^2 + x_-^2) + 2(\hat{p}_0^2 + x_0^2)\big)$$

with hyperbolic resonance $2 : (-1) : 2$ *between the frequencies.*

3. NONCOMMUTATIVE BISYMMETRY ALGEBRA

Now we introduce operators of complex structure $\hat{\xi}_j = \frac{1}{\sqrt{2}}(x_j + i\hat{p}_j)$, $j \in \{+, -, 0\}$, and their adjoint operators $\hat{\xi}_j^*$ in $L^2(\mathbb{R}^3)$, and define the "action" operators $\hat{S}_\pm = \hat{\xi}_\pm^*\hat{\xi}_\pm$, $\hat{S}_3 = \hat{\xi}_0^*\hat{\xi}_0$, and $\hat{S}_0 = 2\hat{S}_+ - \hat{S}_- + 2\hat{S}_3$ whose spectrum consists of numbers multiple of h. Then we have

$$\hat{H}_0 = \frac{\omega_0}{2}(\hat{S}_0 + \frac{3h}{2}).$$

Because the group $\exp\{-it\hat{S}_0/h\}$ is periodic, we apply the quantum averaging procedure

$$U^{-1}\hat{H}U = \hat{H}_0 + \varepsilon\hat{H}_{10} + \varepsilon^2\hat{H}_{20} + O(\varepsilon^3)$$

to pass to the new perturbation operators $\hat{H}_{10}$ and $\hat{H}_{20}$, which commute with the leading part

$$[\hat{H}_0, \hat{H}_{10}] = [\hat{H}_0, \hat{H}_{20}] = 0.$$

Detailed calculations were given in [9].

Lemma 2. *After the averaging procedure, the perturbing Hamiltonian $\hat{H}_1$ from Lemma 1 is transformed to the linear combination*

$$\hat{H}_{10} = \frac{1}{4}\Big(4\hat{A}_+ - 2\hat{A}_- + \hat{A}_0 + \frac{3h}{2}\Big) \tag{6}$$

of the following three commuting operators whose spectrum consists of numbers multiple of h

$$\hat{A}_0 = \hat{S}_-, \quad \hat{A}_+ = \frac{1}{3}\big[2\hat{S}_+ + \hat{S}_3 - \sqrt{2}(\hat{A}_\rho + \hat{A}_\rho^*)\big], \quad \hat{A}_- = \frac{1}{3}\big[\hat{S}_+ + 2\hat{S}_3 + \sqrt{2}(\hat{A}_\rho + \hat{A}_\rho^*)\big]. \tag{7}$$

In this lemma, we have used one of the three generators $\hat{A}_\rho = \hat{\xi}_+^*\hat{\xi}_0$, $\hat{A}_\sigma = \hat{\xi}_+^*(\hat{\xi}_-^*)^2$, $\hat{A}_\theta = (\hat{\xi}_-^*)^2\hat{\xi}_0^*$ of the symmetry algebra of the operator $\hat{H}_0$.

In the Hamiltonian (6), we obtain the new (secondary) resonance $4:(-2):1$ which is ensured by the above-chosen proportion $1:4$ between the axial and longitudinal components of the correction of order ε to the magnetic field. Due to this resonance, we can apply the averaging procedure once again, now to the Hamiltonian $\hat{H}_0 + \varepsilon\hat{H}_{10} + \varepsilon^2\hat{H}_{20}$. We use a unitary operator $\tilde{U}$ to reduce this Hamiltonian to the form

$$\tilde{U}^{-1}(\hat{H}_0 + \varepsilon\hat{H}_{10} + \varepsilon^2\hat{H}_{20})\tilde{U} = \hat{H}_0 + \varepsilon\hat{H}_{10} + \varepsilon^2\hat{H}_{200} + O(\varepsilon^3),$$

where $[\hat{H}_0, \hat{H}_{200}] = [\hat{H}_{10}, \hat{H}_{200}] = 0$.

The twice averaged Hamiltonian $\hat{H}_{200}$ can be written as a function of the joint symmetries of $\hat{H}_0$ and $\hat{H}_{10}$. This bisymmetry algebra is determined by the operators $\hat{A}_0$, $\hat{A}_+$, $\hat{A}_-$ defined in (7) and by the operators

$$\hat{B} = \sqrt{\frac{2}{3}}(\hat{A}_\sigma + \sqrt{2}\hat{A}_\theta). \tag{8}$$

The commutation relations of the generators (7), (8) have the form

$$\begin{gathered}
[\hat{A}_0, \hat{A}_\pm] = [\hat{A}_+, \hat{A}_-] = 0, \\
[\hat{A}_0, \hat{B}] = 2h\hat{B}, \qquad [\hat{A}_+, \hat{B}] = 0, \qquad [\hat{A}_-, \hat{B}] = h\hat{B}, \\
[\hat{B}^*, \hat{B}] = 2h(\hat{A}_0^2 + 4\hat{A}_0\hat{A}_- + 3h\hat{A}_0 + 2h\hat{A}_- + 2h^2),
\end{gathered} \tag{9}$$

together with the conjugate relations. This algebra contains three Casimir elements

$$\hat{D} = 2\hat{A}_- - \hat{A}_0, \qquad \hat{S}_1 = \hat{A}_+, \qquad \hat{K} = \hat{B}\hat{B}^* - 2\hat{A}_0(\hat{A}_0 - h)\hat{A}_-.$$

In realization (7) and (8), the Casimir elements are given by the operators

$$\hat{D} = \frac{4}{3\omega_0}\hat{H}_0 - \frac{4}{3}\hat{H}_{10} + \frac{3h}{2}, \qquad \hat{S}_1 = \frac{1}{3\omega_0}\hat{H}_0 + \frac{2}{3}\hat{H}_{10} - \frac{h}{2}, \qquad \hat{K} = 0.$$

As a result, the twice averaged Hamiltonian $\hat{H}_{200}$ is represented as the quadratic function

$$\hat{H}_{200} = s\Big(\frac{1}{2}(\hat{B} + \hat{B}^*) - a\hat{A}_0^2 - b\hat{A}_0\Big) + \hat{c} \tag{10}$$

in the generators (7) and (8) of the bisymmetry algebra (9). Here we denote

$$\begin{aligned}
s &\simeq \frac{8}{3}k, \qquad a \simeq \frac{1289}{1152}k, \qquad \hat{b} \simeq \frac{1}{576}\Big[1820k\hat{S}_1 - 7k\hat{S}_0 + \frac{540}{k} - 145k + 1896hk\Big], \\
\hat{c} &\simeq \frac{1}{1152}\Big[-580k\hat{S}_1^2 + 104k\hat{S}_1\hat{S}_0 + 7k\hat{S}_0^2 - \Big(\frac{1026}{k} + 1060k + 2244hk\Big)\hat{S}_1 \\
&\quad + \Big(\frac{54}{k} + 290k + 80hk\Big)\hat{S}_0 - \Big(\frac{972h}{k} + 1866h^2k\Big)\Big],
\end{aligned} \tag{11}$$

where k is the ratio of geometric parameters of the trap (3) and the approximate up to $O(\varepsilon)$ values (5) of the parameters ω_0, β, γ are used (because of this, we use the sign $\simeq$ instead of $=$).

Thus we have obtained the following statement.

Lemma 3. *By applying two unitary transformations U and $\tilde{U}$, the original trap Hamiltonian* (2) *is reduced to the form*

$$\frac{\omega_0}{2}\Big(\hat{S}_0+\frac{3h}{2}\Big)+\frac{\varepsilon}{4}\Big(6\hat{S}_1-\hat{S}_0+\frac{3h}{2}\Big)+\varepsilon^2\hat{H}_{200}+O(\varepsilon^3). \tag{12}$$

with the operator $\hat{H}_{200}$ given by (10), (11) *over the algebra* (9). *The action operators $\hat{S}_0$ and $\hat{S}_1$ commute with all generators of the algebra, and their spectrum consists of numbers multiple of h, i.e.,* $\operatorname{Spec}\hat{S}_0=\{hs\mid s\in\mathbb{Z}\}$, $\operatorname{Spec}\hat{S}_1=\{hr\mid r\in\mathbb{Z}_+\}$.

After restriction to the sth eigensubspace of $\hat{S}_0$ and the rth eigensubspace of $\hat{S}_1$, the Hamiltonian (12) *reads as*

$$\frac{1}{3}\Big(s+\frac{3}{2}\Big)h+\frac{\varepsilon}{4}\Big(6r-\frac{2s}{3}+2\Big)h+\varepsilon^2\Big(s\hat{E}+c-\frac{1}{6}\Big(s+\frac{3}{2}\Big)h\Big)+O(\varepsilon^3). \tag{13}$$

Here

$$\hat{E}=\frac{1}{2}(\hat{B}+\hat{B}^*)-a\hat{A}_0^2-b\hat{A}_0$$

and the coefficients b, c are obtained from $\hat{b}$, $\hat{c}$ in (11) *by substituting the numbers sh, rh for the action operators $\hat{S}_0$, $\hat{S}_1$.*

Note that if the control potential W on the ring electrode of the trap is supplemented with a small variation δW so that

$$\frac{\delta W}{W}\approx\varepsilon^2\frac{9}{16}b',$$

then the parameter b in the term linear in $\hat{A}_0$ in the Hamiltonian $\hat{E}$ changes as follows: $b\to b+b'$ (also, an insignificant constant is added to $\hat{c}$). Thus (see [11]), varying the potential W in the order ε^2, we can strongly vary the parameter b; in particular, we can change its sign.

4. AVOIDED CROSSING FOR THE TOP HAMILTONIAN OVER A NON-LIE ALGEBRA

We have reduced the model of planar resonance Penning trap to the top-like Hamiltonian $\hat{E}=(1/2)(\hat{B}+\hat{B}^*)-a\hat{A}_0^2-b\hat{A}_0$ with known numerical coefficients a and b over the algebra

$$\begin{gathered}[\hat{A}_0,\hat{A}_-]=0,\qquad [\hat{A}_0,\hat{B}]=2h\hat{B},\qquad [\hat{A}_-,\hat{B}]=h\hat{B},\\ [\hat{B}^*,\hat{B}]=2h(\hat{A}_0^2+4\hat{A}_0\hat{A}_-+3h\hat{A}_0+2h\hat{A}_-+2h^2)\end{gathered} \tag{14}$$

with Casimir elements $\hat{D}=2\hat{A}_--\hat{A}_0$ and $\hat{K}=\hat{B}\hat{B}^*-2\hat{A}_0(\hat{A}_0-h)\hat{A}_-$. In the discussed model, we are dealing only with the irreducible representation of this algebra, where the operator $\hat{D}=\hat{S}_0-2\hat{S}_1+2h$ takes the value $d=(s-2r+2)h$ and the element $\hat{K}$ takes the value zero.

The Poisson algebra is given by the relations

$$\{A_0,B\}=2iB,\qquad \{\bar{B},B\}=2iA_0(3A_0+2d). \tag{15}$$

The desired irreducible representation corresponds to the symplectic leaf determined by the equations

$$\begin{cases}Y_1^2+Y_2^2=A_0^2(A_0+d),\\ A_0>0,\quad A_0\geq -d.\end{cases} \tag{16}$$

Here we use the notation $B=Y_1+iY_2$.

Let us see how the spectral lines of the Hamiltonian $\hat{E}$ depend on variations of the numerical parameter b in the semiclassical approximation ($0<h\ll 1$).

The corresponding classical mechanical system with Hamiltonian

$$E=Y_1-aA_0^2-bA_0$$

is defined on the two-dimensional symplectic leaf (16) with the canonical (Kirillov) symplectic form ω.

The symplectic leaf (16) is a surface of rotation around the axis A_0 in the enveloping three-dimensional space with coordinates (Y_1, Y_2, A_0). In the case $d \le 0$, the symplectic leaf is a smooth cup-shaped surface with minimum at the point $A_0 = -d$, and in the case $d > 0$, the symplectic leaf is shaped as a cusp with the singularity at the origin (see Fig. 1).

The trajectories of the classical motion corresponding to the energy $E = \mathcal{E}$ can be obtained as intersections of the symplectic leaf with the level surfaces of the Hamiltonian E in the three-dimensional space (Y_1, Y_2, A_0). Figure 1 shows the cross-section of the symplectic leaf (16) by the plane $Y_2 = 0$ and the family of level lines of the Hamiltonian E.

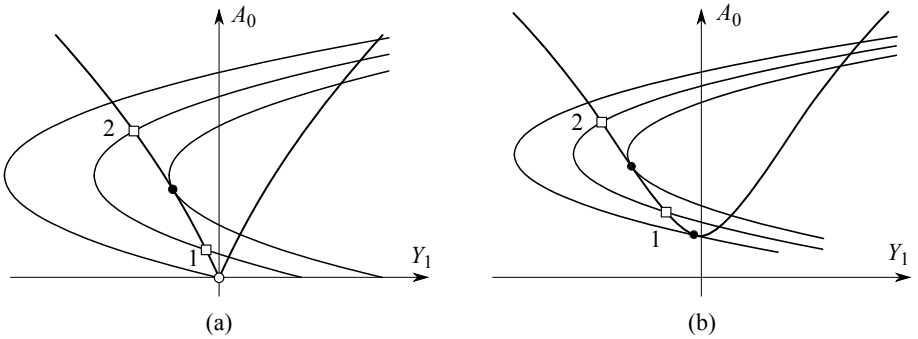

Fig. 1. Figures (a) and (b) show the cross-section of the symplectic leaf by the plane $Y_2 = 0$ in the cases of "cusp" and "cup," respectively. The figures also show three parabolas, i.e., curves of constant energy $E = \mathcal{E}$. The left parabola corresponds to $\mathcal{E}_{min}$, the middle parabola corresponds to the "double-well" regime, and the right parabola corresponds to $\mathcal{E} = \mathcal{E}_{max}$, i.e., to the unstable equilibrium and the separatrix. The small squares with indexes 1 and 2 are the turning points M_1 and M_2 on the classical trajectories γ_1 and γ_2, respectively.

By analyzing Fig. 1, we obtain the following statement.

Lemma 4. *If the parameter $b < 0$ is sufficiently large in absolute value, then there is a separatrix separating pairs of trajectories of the periodic motion corresponding to the same energy level $\mathcal{E}$. In the case of "cusp" ($d > 0$), the condition for origination of such pairs of trajectories is simple:*

$$b < 0, \qquad b^2 > d > 0.$$

In the case of "cup" ($d \le 0$), the pairs of trajectories of periodic motion corresponding to the same energy level $\mathcal{E}$, also arise for a sufficiently large in absolute value parameter $b < 0$.

The quantum energy levels which approximate the discrete spectrum of the Hamiltonian $\hat{E}$ up to $O(h^2)$ can be determined by using the Planck–Bohr–Sommerfeld quantization rule

$$\frac{1}{2\pi}\int_{\Sigma} \omega = h(n + 1/2), \tag{17}$$

where n is an integer, Σ is the bounded domain in the symplectic leaf with the boundary $\partial\Sigma = \gamma$ and γ is a trajectory of periodic motion corresponding to the energy $E = \mathcal{E}$. Solving (17) as an equation for the energy $\mathcal{E}$ for different quantum numbers n, we obtain a series of energy levels $\mathcal{E}^{(n)}$.

Let us mention, that the singularity of the Kirillov form ω at zero appearing in the "cusp" case is integrable, and the rule (17) still works in this case.

If the parameters of the system are chosen so that in a certain interval $(\mathcal{E}_{min}, \mathcal{E}_{max})$ each energy level $\mathcal{E}$ consists of a pair of periodic trajectories γ_1 and γ_2 of classical motion, then in this interval there are two series $\mathcal{E}_1^{(n)}$ and $\mathcal{E}_2^{(m)}$ determined separately over the curves γ_1 and γ_2 by the Planck–Bohr–Sommerfeld rule (17) with quantum numbers n and m. For definiteness, we assume that γ_1 is the trajectory corresponding to lesser values of A_0, and γ_2 is the trajectory corresponding to greater values of A_0.

The trajectories γ_1 and γ_2 are represented by two segments of the middle parabola on Fig. 1. Let M_j be the point of intersection of the trajectory γ_j with the plane $Y_2 = 0$ at $Y_1 < 0$, $j = 1, 2$. They are labeled by indices 1 and 2 on Fig. 1.

Such a geometric picture is similar to the one arising when the Hamiltonian $p^2 + V(x)$ is considered on the straight line with the double-well potential $V(x)$. In the problem under study, for definiteness, we also call this regime a "double-well" regime.

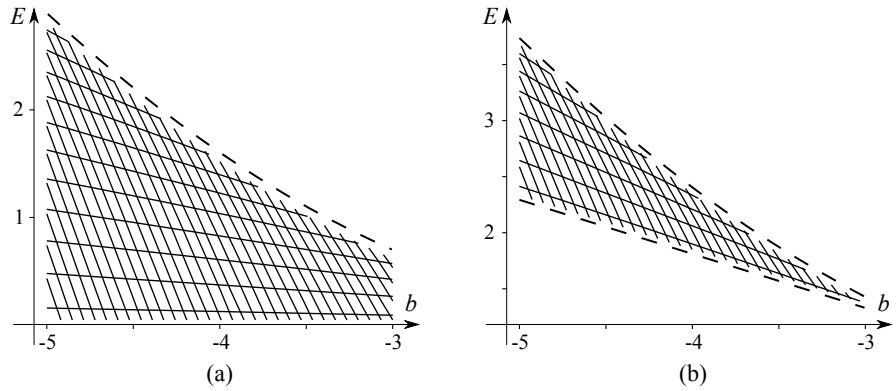

Fig. 2. Figures (a) and (b) show the grid of approximate energy levels of the operator $\hat{E}$ between the lines $\mathcal{E}_{min}$ and $\mathcal{E}_{max}$ for the parameters $b \in [-5, -3]$, $a = 1$, $h = 1/30$. Figure (a) illustrates the "cusp" case for $d = 1$, and Fig. (b) illustrates the "cup" case for $d = -1/2$. The dashed lines correspond to $\mathcal{E}_{min}$ and $\mathcal{E}_{max}$, the sloping lines of the grid correspond to γ_1, and the abrupt lines, to the trajectories γ_2.

Figures 2 present the dependence of the approximate energy levels $\mathcal{E}_1^{(n)}$ and $\mathcal{E}_2^{(m)}$ on the parameter b in the interval $(\mathcal{E}_{min}, \mathcal{E}_{max})$ both in the "cusp" and "cup" cases. In the "cusp" case, the minimal energy $\mathcal{E}_{min} = 0$ corresponds to the trajectory passing through the singularity at the origin, and $\mathcal{E}_{max}$ is the energy corresponding to the separatrix. In the "cup" case, the minimal energy $\mathcal{E}_{min}$ corresponds to the stable equilibrium, and $\mathcal{E}_{max}$, as in the "cusp" case, corresponds to the separatrix (see Fig. 1).

Lemma 5. *The curves of approximate energy levels $\mathcal{E}_1^{(n)}$ and $\mathcal{E}_2^{(m)}$ form a grid with many intersections in the interval $(\mathcal{E}_{min}, \mathcal{E}_{max})$, where the levels $\mathcal{E}_1^{(n)}$ intersect with $\mathcal{E}_2^{(m)}$ for different n and m. Since the parameter h is small, the energy curves $\mathcal{E}_1^{(n)}$ with different values of the quantum number n are practically parallel and lie at the distance of order h from each other. The family of curves $\mathcal{E}_2^{(m)}$ have a similar structure.*

The methods of semiclassical approximation [14] allow one to construct normalized approximate stationary states $\psi_1^{(n)}$ and $\psi_2^{(m)}$ for each energy level $\mathcal{E}_1^{(n)}$ and $\mathcal{E}_2^{(m)}$, and these states satisfy the spectral equation

$$\hat{E}\psi = \mathcal{E}\psi$$

with a small discrepancy of order $O(h^2)$. The states $\psi_1^{(n)}$ and $\psi_2^{(m)}$ are localized in small neighborhoods of the classical trajectories γ_1 and γ_2, respectively (in the sense that corresponding Wigner or Husimi distributions are concentrated there up to $O(h^\infty)$).

If for a fixed value of the parameter b, we consider the energy level $\mathcal{E}_1^{(n)}$ at a far enough distance from its points of intersection with the levels $\mathcal{E}_2^{(m)}$, then we can claim that the exact stationary state of the Hamiltonian $\hat{E}$ is close to $\psi_1^{(n)}$ and is, therefore, localized in a neighborhood of only one of the two trajectories of classical motion. The same holds for the levels $\mathcal{E}_2^{(m)}$ and the states $\psi_2^{(m)}$. The picture is essentially different in a neighborhood of the points of intersection of the approximate energy levels $\mathcal{E}_1^{(n)}$

and $\mathcal{E}_2^{(m)}$. Since the discrete spectrum of the operator $\hat{E}$ is nondegenerate, it follows that the so-called effect of avoided crossing of energy levels occurs [15], [16].

We obtain the following statement.

Theorem 1. *In the "double-well" regime, i.e., under conditions of Lemma 4, two energy levels of the top Hamiltonian $\hat{E}$ come at the minimal distance ΔE from each other for some critical value of the parameter $b = b^*_{m,n}$ and then go away from each other as b increases. The stationary states corresponding to the minimal distance ΔE between energy levels have the form of a symmetric and an antisymmetric combination of the states $\psi_1^{(n)}$ and $\psi_2^{(m)}$:*

$$\frac{1}{\sqrt{2}}\big(\psi_1^{(n)} \pm \psi_2^{(m)}\big), \tag{18}$$

i.e., both stationary states are uniformly localized near the trajectories γ_1 and γ_2.

The obtained bilocalization on pairs of closed curves for the top Hamiltonian over the symmetry algebra generates the bilocalization of quantum states of the electron on pairs of 3D-tori in the phase space of the Penning trap.

About stationary states of the form (18) we say that they are bilocalized [12], [17]. It is assumed that the phases of wave functions of the states $\psi_1^{(n)}$ and $\psi_2^{(m)}$ are chosen so that they are consistent; otherwise, an additional phase multiplier $e^{i\phi}$ in front of $\psi_2^{(m)}$ can arise in formula (18).

The appearance of avoided crossing of the spectral levels and bilocalized stationary states are a well-known quantum effect (see, e.g., [15], [18], [19]) related to the possibility of quantum tunneling of a state between trajectories of classical motion γ_1 and γ_2. At a far distance from points of avoided crossing, the quantum tunneling is practically not manifested, and the state remains localized near one of the trajectories. On the other hand, in a small neighborhood of points of avoided crossing of energy levels, the exponentially small effects of quantum tunneling significantly (of the order 1) influence the wave functions of stationary states. A sharp variation of the tunneling dynamics in a quantum system due to a variation of the external parameter is known as the *effect of resonant tunneling*.

The key role in the description of the effect of avoided crossing of energy levels is played by a small value ΔE, which is called the *value of tunnel splitting* or the *tunneling amplitude*. For example, if the parameter of a system is tuned at the avoided crossing value $b = b^*_{m,n}$ and the initial quantum state is localized in a neighborhood of only one closed trajectory of the classical motion, then during the time $\pi h/\Delta E$ the state completely tunnels into a neighborhood of the other classical trajectory at the same energy level, then returns, and so on. Thus, the quantity $\Delta E/h$ plays the role of frequency of tunnel transitions.

As is well known, the tunneling effects are exponentially small in the parameter h of the semiclassical approximation. The value of the tunnel energy splitting ΔE usually has an exponential asymptotics like

$$\Delta E = \exp\left(-\frac{1}{h}S + O(1)\right). \tag{19}$$

Below we present a formula for the exponent S in the case of the quantum top $\hat{E}$ over the non-Lie algebra (14).

5. TUNNEL SPLITTING, COMPLEXIFICATION, AND INSTANTON

It is known that the description of tunneling dynamics of a quantum particle in the semiclassical approximation is closely related to the complexification of classical Hamiltonian equations (see the survey in [20], [21]).

Let us consider the natural complexification of the Poisson algebra (15) and the Hamiltonian E under the assumption that the coordinates Y_1, Y_2, A_0 take complex values. Then the complexification of the Hamilton system, the symplectic leaf (16), and the symplectic structure on the leaf also arise.

We shall consider only the domain of the complexification where the real part of A_0 is nonnegative and $Re\, A_0 \geq -d$ in the "cup" case where $d < 0$.

Definition 1. Periodic trajectories of the complexified Hamilton system with pure imaginary time that intersect the real symplectic leaf are called *symplectic instantons*.

Each symplectic instanton necessarily lies in the complexification of the symplectic leaf (16) and belongs to a constant energy level of the complexified Hamiltonian E. In the "double-well" regime symplectic instantons automatically interset both the real trajectories γ_1 and γ_2 belonging to the given energy level $E = \mathcal{E}$.

Theorem 2. *In the "double-well" regime, suppose that the energy $\mathcal{E}$ and the parameter b are in $O(h^2)$-neighborhood of the avoided crossing values. Then the avoided crossing energy splitting ΔE, i.e., the minimal gap between the two energy levels of the Hamiltonian $\hat{E}$ over the algebra* (14)*, has the asymptotics* (19)*, where the tunneling action S is given by the following geometric formula:*

$$S = \frac{1}{2i}\int_{\tilde{\Sigma}} \omega. \tag{20}$$

Here $\tilde{\Sigma}$ is a membrane in the complexified symplectic leaf whose boundary $\partial\tilde{\Sigma} = \tilde{\gamma}$ is the symplectic instanton intersecting the real trajectories γ_1 and γ_2 at points where $Y_2 = 0$ and $Y_1 < 0$, i.e., at the points M_1 and M_2 (see Figs. 1*).*

Remark 1. Although the idea of instanton first arose in the study of the low-lying quantum states tunneling between two stable equilibrium points [22], [23], the same terminology is applied in the case of tunneling between Lagrangian submanifolds on upper energy levels [24].

Usually (see [20], [25]), the instanton is understood as half the trajectory $\tilde{\gamma}$, i.e., a path whose initial and end points lie on different trajectories of the classical motion. The use of the complete instanton as a periodic trajectory allows us to obtain the invariant geometric formula such as (20) based on the symplectic structure (15) alone.

Note that in this formula the value of the integral depends on the instanton homotopic class only, and thus the closed curve $\tilde{\gamma}$ in (20) can be arbitrarily deformed inside the given energy level. Such a topological point of view was used in [21] for the description of tunnel splitting in the case of the Laplace–Beltrami operator.

Proof of Theorem 2. The proof uses some functional analysis related to the difference operator appearing in the natural representation of the top Hamiltonian $\hat{E}$. The details of this analysis can be recovered by following, for instance, the approach of [26]. Here we present, step by step, a scheme for the derivation of formula (20) and demonstrate the existence of the symplectic instanton.

The method for calculating the tunnel splitting ΔE is based on the consideration of the spectral problem for the operator $\hat{E}$ in the spectral representation of the operator $\hat{A}_0$. For convenience, we introduce the coordinate $\hat{q} = \hat{A}_0/2$ and the operator $\hat{p} = -ih\partial_q$.

Since

$$\hat{B} \circ q = (q - h) \circ \hat{B},$$

we see that the operator $\hat{B}$ in this representation becomes

$$\hat{B} = \beta(q, h)e^{-i\hat{p}},$$

where $\beta(q, h)$ is a real function. The explicit expression for this function can be found by substituting the operator $\hat{B}$ into the formula for the Casimir operator $\hat{K} = 0$; doing this, we obtain

$$\beta(q, h) = 2\sqrt{q(q - h/2)(2q + d)} = 2q\sqrt{2q + d} + O(h).$$

In this representation, the spectral problem for the operator $\hat{E}$ takes the form of the following Hermitian three-term recurrence relation:

$$\frac{1}{2}\beta(q + h, h)y(q + h) - \left(4a\,q^2 + 2b\,q\right)y(q) + \frac{1}{2}\beta(q, h)y(q - h) = \mathcal{E}y(q), \tag{21}$$

where $y(q)$ is the wave function of the stationary state. The variable q takes values of the form $q_0 + hl$, $l \in \mathbb{Z}_+$ over the spectrum of $\hat{A}_0/2$, and the explicit form of q_0 depends on the representation in question, i.e., on the numbers r and s in (13):

$$q_0 = \begin{cases} 0, & s \geq 2r-2, \quad s \text{ even}; \\ h/2, & s \geq 2r-2, \quad s \text{ odd}; \\ (2r-2-s)h/2, & s < 2r-2. \end{cases}$$

WKB methods similar to the corresponding methods for differential equations have been developed for three-term recurrence relations of the form (21); see, e.g., [26]–[29]. In [30]–[33], the discrete WKB method was also used in problems of estimating tunneling effects.

The transition formulas from the coordinates (q,p) on the symplectic leaf (16) to the coordinates (Y_1, Y_2, A_0) have the form

$$A_0 = 2q, \qquad Y_1 = 2q\sqrt{2q+d}\cos(p), \qquad Y_2 = -2q\sqrt{2q+d}\sin(p). \tag{22}$$

Therefore, the classical Hamiltonian E in the coordinates (q,p) reads

$$E(q,p) = 2q\sqrt{2q+d}\,\cos(p) - 4a\,q^2 - 2b\,q. \tag{23}$$

The turning point for the Hamiltonian (23) is determined as the point q where the velocity is equal to zero

$$\dot{q} = \frac{\partial E}{\partial p} = -2q\sqrt{2q+d}\,\sin(p) = 0.$$

Hence there are two types of regular turning points, namely, the points with $p = 0$ and $p = \pi$. Substituting $p = 0$ and $p = \pi$ into the equation $E = \mathcal{E}$, we obtain the following equation for the coordinates of the turning points:

$$\frac{\mathcal{E} + 4a\,q^2 + 2b\,q}{2x\sqrt{2q+d}} = \pm 1,$$

where the "+" sign corresponds to $p = 0$ and the "−" sign corresponds to $p = \pi$. Figures 3 show the coordinates of the turning points depend on the energy $\mathcal{E}$.

We see that (for values of the parameter b belonging to intervals described above) the regions of classical motion form a "double-well" structure with a barrier separating the classical trajectories γ_1 and γ_2.

We assume that the values of energy $\mathcal{E}$ correspond to the "double-well" regime so that the barrier (forbidden region) is located between the turning points q_1 and q_2, as is shown in Figs. 3. Figures 3 clearly demonstrate that turning points q_1 and q_2 are corresponds to the momentum $p = \pi$.

By applying methods [27]–[33], as well as the approach of [26], to our problem, we obtain the following result.

Lemma 6. *For the spectral problem* (21) *the tunneling action S has the standard form as in the case of the Schrödinger equation with double-well potential:*

$$S = \operatorname{Im}\int_{q_1}^{q_2} p(q,\mathcal{E})\,dx = \int_{q_1}^{q_2} \operatorname{arccosh}\left(-\frac{\mathcal{E} + 4a\,q^2 + 2b\,q}{2q\sqrt{2q+d}}\right)\,dq,$$

where $\operatorname{arccosh}(z) = \ln(z + \sqrt{z^2-1}) > 0$ *for* $z > 1$ *and the momentum $p(q,\mathcal{E})$ is the complex branch of the solution to the equation $E(q,p) = \mathcal{E}$.*

The quantity S can now be written in an invariant form independent of the specific choice of coordinates on the symplectic leaf. Indeed, S has the form

$$S = \frac{1}{2i}\oint_{\tilde{\gamma}} p\,dx, \tag{24}$$

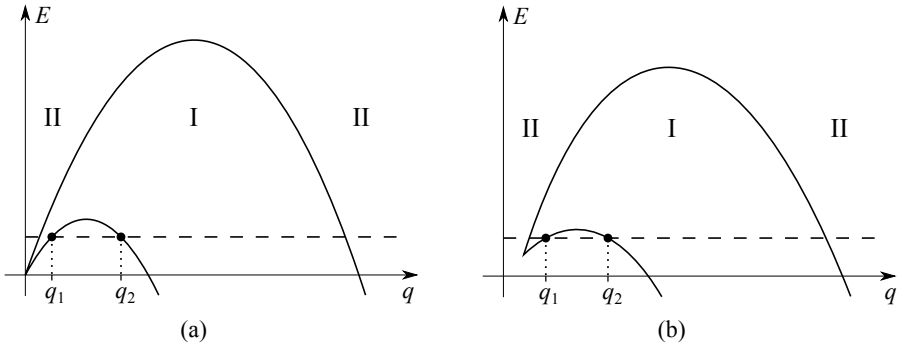

Fig. 3. Figures (a) and (b) show the turning points of the Hamiltonian $E(x,p)$ depending on the energy in the "cusp" and "cup" cases, respectively. The small and big parabolic-like curves correspond to $p=\pi$ and $p=0$ turning point curves, respectively. The dashed line shows the energy corresponding to the "double-well" regime. Region I is classically allowed, and regions II are classically forbidden. The figures show the turning points q_1 and q_2 determining the barrier between two classically allowed regions.

where $\tilde{\gamma}$ is the trajectory of the periodic motion in the complexified Hamiltonian system

$$\frac{dq}{d\tau}=-i\frac{\partial E}{\partial p},$$
$$\frac{dp}{d\tau}=i\frac{\partial E}{\partial q},$$

which corresponds to a motion with pure imaginary time $t=-i\tau$.

The trajectory $\tilde{\gamma}$ starts at $\tau=0$ at the turning point $q=q_1$, $p=\pi$ on the curve γ_1, and then moves towards the turning point $q=q_2$, $p=\pi$ on the curve γ_2. These turning points are M_1 and M_2, shown in Fig. 1. On the trajectory $\tilde{\gamma}$, the value $E(q,p)=\mathcal{E}$ remains unchanged, the coordinate q takes real values from q_1 to q_2, and the coordinate p takes complex values of the form $p(\tau)=\pi+i\tilde{p}(\tau)$. Thus, the trajectory $\tilde{\gamma}$ is a symplectic instanton, i.e., it lies on the complexification of the Lagrangian manifold $E(q,p)=\mathcal{E}$ and connects two real trajectories γ_1 and γ_2 belonging to this submanifold.

The quantity S in formula (24) is written in terms of the complexification of the coordinates q and p on the symplectic leaf. We note that the Kirillov symplectic form on the leaf (16) is given by $\omega=dp\wedge dq$, and that the orientation of the instanton $\tilde{\gamma}$ in (24) agrees with the orientation induced by the symplectic form. Thus, applying Stokes' theorem, we can transform formula (24) to the form (20).

In the initial Poisson coordinates (Y_1,Y_2,A_0), the symplectic instanton $\tilde{\gamma}$ can be chosen so that it passes through the points M_1 and M_2 of the real trajectories γ_1 and γ_2 at which $Y_2=0$ and $Y_1<0$. On this symplectic instanton, the coordinates A_0 and Y_1 remain real and the coordinate Y_2 takes pure imaginary values.

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