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Instantons via Breaking Geometric Symmetry in Hyperbolic Traps*

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Abstract—Using geometrical and algebraic ideas, we study tunnel eigenvalue asymptotics and tunnel bilocalization of eigenstates for certain class of operators (quantum Hamiltonians) including the case of Penning traps, well known in physical literature. For general hyperbolic traps with geometric asymmetry, we study resonance regimes which produce hyperbolic type algebras of integrals of motion. Such algebras have polynomial (non-Lie) commutation relations with creation-annihilation structure. Over this algebra, the trap asymmetry (higher-order anharmonic terms near the equilibrium) determines a pendulum-like Hamiltonian in action-angle coordinates. The symmetry breaking term generates a tunneling pseudoparticle (closed instanton). We study the instanton action and the corresponding spectral splitting.

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1. INTRODUCTION

In order to trap in a local place of physical 3D-space and hold a single charge particle, one can use a homogeneous magnetic field (which rotates the charge in the perpendicular plane) and an electric potential (which provides stability along the magnetic axis). Since the potential obeys the Laplace equation, its quadratic part near the equilibrium point must be of saddle type, not elliptic. Thus, the normal form of the trap Hamiltonian is a linear combination of oscillators (action operators) with different signs of coefficients. Among examples of such hyperbolic traps are the well-known Penning traps [1]–[4], which become very interesting controllable quantum devices in nano-scale. The eigenvalue problem for the corresponding quantum Hamiltonian is especially profound under frequency resonance.

In the resonance regime, such a trap Hamiltonian generates a noncommutative and nonlinear (non-Lie) algebra of hyperbolic type, with infinite dimensional irreducible representations. The corresponding Poisson algebra has noncompact symplectic leaves. The dynamics on these leaves comes from the anharmonic part of the trap potential.

Often this anharmonic part (whose existence is unavoidable for technological reasons) is regarded as an injury and nuisance characteristic of the device. But, at the same time, this part can be used for creation and control of exclusive states and quasiparticles in irreducible representations of the algebra of integrals of motion of the trapped charge. For instance, one can expect to see multilocalized eigenstates created by tunneling pseudoparticles (instantons). These quantum phenomena in the trap are accompanied by very interesting classical dynamics, symplectic geometry, and topology.

Let us stress that the principal role is played by resonance of normal frequencies of the harmonic part (of the "ideal" Penning trap). Without resonance, the anharmonic part does not generate any phenomena of this kind.

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In this note, our guiding example of hyperbolic trapping system is a planar rectangular Penning trap with $3:(-1)$ resonance between the modified cyclotron and the magnetron frequencies [5]. The trap geometric asymmetry, i.e., the deviation of the rectangle electrodes from square shape, generates instantons and creates a 2-level quantum subsystem after suitable tuning electric voltage on the trap electrodes. We analyze how to generalize this particular example to higher resonances in a wide class of hyperbolic traps. The breaking symmetry source generating instantons in general case is a higher anharmonism (of the trap) whose order corresponds to the order of resonance.

In Sec. 2, we consider a general type polynomial Hamiltonian (2.2) over the Heisenberg algebra (2.1). The harmonic part (2.3) is assumed to be at resonance (2.7). Then the Hamiltonian is reduced to the form (2.14) over the algebra (2.11). In Sec. 3, the original problem is replaced by a spectral problem for the Hamiltonian (3.1). In Sec. 4, we introduce an irreducible representation of the algebra (2.11) by the "action-angle" operators (4.1) and reduce the spectral problem to the difference equation (4.2). In Sec. 5 (Theorem 1 and Corollary 1), we state the basic results about tunneling effects for this difference equation as well as for the original polynomial Hamiltonian (2.2). In Sec. 5, Theorem 2, we deal with the non-polynomial case under the specific resonance $3:(-1)$ for energy levels in a "mezzo-classical" zone.

2. HYPERBOLIC TRAPS

In a Hermitian representation of the Heisenberg algebra with four generators $\hat z = (\hat z_+, \hat z_-)$ and two nontrivial commutation relations

$$[\hat z_\alpha, \hat z_\alpha^*] = \hbar \qquad (\alpha = +, -), \tag{2.1}$$

let us consider the self-adjoint operator $\mathbb{H} = \mathcal{H}(\hat z^* | \hat z)$ whose Wick symbol $\mathcal{H}$ is given by a sum of homogeneous functions in $(\bar z, z)$-coordinates

$$\mathcal{H} = \frac{1}{\hbar}(H_0 + H_1 + H_2 + \dots + H_N), \qquad \deg H_j = j + 2, \quad N \geq 2. \tag{2.2}$$

Under the assumption that normal frequencies of the harmonic part H_0 are in resonance, our goal is to study the spectral problem for the operator $\mathbb{H}$ in the semiclassical approximation $\hbar \to 0$, in particular, to investigate the opportunity to observe the effect of tunneling splitting of its eigenvalues and multilocalization of corresponding eigenstates. We intend to find conditions for the existence of its semiclassical bi-states in the sense of [5] and investigate the corresponding instanton geometry.

We assume that the harmonic summand H_0 is just the hyperbolic oscillator

$$H_0(\bar z | z) = \omega_+ \bar z_+ z_+ - \omega_- \bar z_- z_- \tag{2.3}$$

with two frequencies $\omega_\pm > 0$.

The quantum operators $\hat z_\pm^* \hat z_\pm$ have the spectra $\{\hbar n_\pm \mid n_\pm = 0, 1, 2, \dots\}$ and thus the eigenvalues of the quantized oscillator (2.3) have the form $\pm \hbar \omega(n)$, where $\omega(n) \stackrel{\text{def}}{=} |\omega_+ n_+ - \omega_- n_-|$. Suppose that

$$1 \ll \omega(n) \ll \hbar^{-1}. \tag{2.4}$$

This inequality means that we deal with the semiclassical situation $\hbar \ll 1$ in (2.1) and consider the intermediate eigenstates of the oscillator, i.e., not the lowest ones (closest to zero) and not too excited. Let us introduce the parameter $\varepsilon \stackrel{\text{def}}{=} \hbar \omega(n)$, then

$$\hbar \ll \varepsilon \ll 1. \tag{2.4a}$$

In the normalized generators $\hat a_\pm \stackrel{\text{def}}{=} \hat z_\pm / \sqrt{\varepsilon}$, we obtain the Hamiltonian

$$\mathbb{H} = \frac{1}{h} \sum_{j \geq 0} \varepsilon^{j/2} H_j(\hat a^* | \hat a) \tag{2.5}$$

over the algebra with canonical relations

$$[\hat a_\pm, \hat a_\pm^*] = h, \tag{2.6}$$

where $h \overset{\text{def}}{=} \hbar/\varepsilon$ is the effective semiclassical parameter, since $h \ll 1$, due to (2.4a).

The Hamiltonian (2.5) has the leading part determined by the hyperbolic oscillator $\hat{H}_0 = H_0(\hat{a}^*|\hat{a})$ as well as the perturbing part $\sqrt{\varepsilon}\hat{H}_1 + \varepsilon\hat{H}_2 + \dots$.

If the frequencies ω_+ and ω_- in (2.3) are not at resonance, then the averaging procedure reduces the perturbing part just to a function in two mutually commuting "actions" $\hat{S}_\pm \overset{\text{def}}{=} \hat{a}^*_\pm \hat{a}_\pm$. In such a case, the Hamiltonian does not admit any instantons (near the zero energy level).

Now let us assume that the frequencies in (2.3) are in the resonance

$$\omega_+ : \omega_- = k_+ : k_- \qquad (k_\pm \in \mathbb{N}). \tag{2.7}$$

In this case, up to an arbitrary accuracy ε^N, the averaging reduces (2.5) to a commutative form in which the perturbing part commutes with the leading term $\hat{H}_0$.

The algebra of operators commuting with $\hat{H}_0 = \omega_+\hat{S}_+ - \omega_-\hat{S}_-$ is generated by the action operators $\hat{S}_\pm$ and also by the operator $\hat{B} = (\hat{a}^*_+)^{k_-}(\hat{a}^*_-)^{k_+}$ and its conjugation $\hat{B}^*$. The commutation relations between them are the following (see in [6]–[8])

$$[\hat{S}_\pm, \hat{B}] = h\, k_\mp \hat{B}, \qquad [\hat{B}^*, \hat{B}] = h\, r_h(\hat{S}_+, \hat{S}_-). \tag{2.8}$$

Here the polynomial r_h is determined by

$$r_h(s_1, s_2) \overset{\text{def}}{=} \frac{1}{h}(g_h(s_1 + k_- h, s_2 + k_+ h) - g_h(s_1, s_2)),$$

where g_h is given by

$$g_h(s_1, s_2) \overset{\text{def}}{=} \prod_{j_1=0}^{k_- -1}(s_1 - j_1 h) \cdot \prod_{j_2=0}^{k_+ -1}(s_2 - j_2 h). \tag{2.9}$$

This algebra has the Casimir elements

$$\hat{K} = \hat{B}\hat{B}^* - g_h(\hat{S}_+, \hat{S}_-), \qquad \hat{C} = k_+\hat{S}_+ - k_-\hat{S}_-. \tag{2.10}$$

In our representation, the first element equals zero: $\hat{K} = 0$.

Only in the case $k_+ = k_- = 1$, i.e., in the case of $1 : (-1)$ resonance in the oscillator (2.3), the algebra (2.8) is of Lie type. For all other resonances, the polynomial r_h in (2.8) is of degree ≥ 2 and, therefore, (2.8) is not a Lie algebra. This type of polynomial algebra has a well-developed representation theory [9], [10].

Let us restrict ourselves to the eigensubspace of the Casimir element $\hat{C} = \frac{k_-}{\omega_-}\hat{H}_0$ with the eigenvalue k_-/ω_-, i.e., to the subspace of $\hat{H}_0$ corresponding to the eigenvalue 1. Denote[1] $\hat{A} = \hat{S}_-/k_+$. Then algebra (2.8) is reduced to

$$[\hat{A}, \hat{B}] = h\hat{B}, \qquad [\hat{B}^*, \hat{B}] = h\rho_h(\hat{A}) \tag{2.11}$$

with the Casimir element (2.10)

$$\hat{K} = \hat{B}\hat{B}^* - \varphi_h(\hat{A}). \tag{2.12}$$

Here $\rho_h(a) = (\varphi_h(a + h) - \varphi_h(a))/h$, and the polynomial $\varphi_h(a) = g_h(k_-\, a + 1/\omega_+, k_+\, a)$ is obtained from (2.9).

In the irreducible representation of the algebra (2.11), the spectrum of $\hat{A}$ is given by an h-step arithmetic sequence $a_m, a_m + h, a_m + 2h, \dots$, whose base a_m is chosen from the finite set

$$\left\{ \frac{hm}{k_+} \;\middle|\; m = 0, 1, \dots, k_+ - 1 \right\}.$$

[1]On the eigensubspace of $\hat{H}_0$, corresponding to the eigenvalue -1, one needs to choose $\hat{A} = \hat{S}_+/k_-$ and redefine the function φ_h in (2.12).

Thus, via shifting the operator $\hat{A}$ and the argument of the function φ_h by the constant a_m, we can assume without loss of generality that the spectrum of $\hat{A}$ is given by $\{0, h, 2h, \dots\}$.

Now let us return to the Hamiltonian (2.5). By applying the operator averaging to its anharmonic terms, we project them into the irreducible representation of the algebra (2.11). For a detailed description of the operator averaging procedure in resonance cases, see [5]–[8], [11]. In the case of resonance $2:(-1)$, the averaging applied to (2.5) yields

$$\mathbb{H} \sim \frac{1}{h}(\hat{H}_0 + \sqrt{\varepsilon}(\mu\hat{B} + \bar{\mu}\hat{B}^*) + O(\varepsilon)) \tag{2.13}$$

with a number μ determined by the coefficients of the third-degree polynomial H_1 in $(\bar{z}, z)$-coordinates. Since the spectrum of $\mu\hat{B} + \bar{\mu}\hat{B}^*$ in (2.13) is continuous and unbounded (if $\mu \neq 0$), this resonance produces a local instability of the dynamics. This situation is out of the scope of our present analysis.[2]

In the case of resonance $3:(-1)$, the averaging implies

$$\mathbb{H} \sim \frac{1}{h}\bigg(\hat{H}_0 + \varepsilon\bigg(\frac{\mu}{2}\hat{B} + \frac{\bar{\mu}}{2}\hat{B}^* + \alpha\hat{A}^2 + \beta\hat{A} + \gamma\bigg) + O(\varepsilon^2)\bigg) \tag{2.14}$$

with some numbers μ, α, β and γ determined by the coefficients of the third- and fourth-degree polynomials H_1 and H_2 in $(\bar{z}, z)$-coordinates [5].

For higher-order resonances (2.7) with $k_+ + k_- \geq 5$, the averaging provides the same-type effective Hamiltonian (2.14) with coefficient μ of order $\varepsilon^{(k_+ + k_- - 4)/2} = O(\sqrt{\varepsilon})$ determined by higher-order anharmonic terms in (2.2). Below we shall analyze an operator of this type.

3. SYMPLECTIC LEAVES AND TRAJECTORIES

Without loss of generality, we consider the Hamiltonian

$$\hat{E} = \frac{\mu}{2}(\hat{B} + \hat{B}^*) + \alpha\hat{A}^2 + \beta\hat{A}, \qquad \mu > 0, \tag{3.1}$$

with known numerical coefficients over the polynomial algebra (2.11) in the representation where the Casimir operator (2.12) equals zero: $\hat{K} = 0$.

In the classical limit as $h \to 0$, instead of the quantum Hamiltonian (3.1), we deal with the corresponding mechanical system with Hamiltonian $E = \mu Y_1 + \alpha A^2 + \beta A$ over the Poisson algebra

$$\{Y_2, Y_1\} = \frac{1}{2}\rho_0(A), \qquad \{A, Y_1\} = Y_2, \qquad \{A, Y_2\} = -Y_1, \tag{3.2}$$

where $B = Y_1 - iY_2$. The symplectic leaf $K = 0$ is the algebraic surface of revolution:

$$Y_1^2 + Y_2^2 = \varphi_0(A). \tag{3.3}$$

Classical trajectories can be obtained as intersections of the symplectic leaf with the parabolic cylinder of the energy surface $\{E = \mathcal{E}\}$, i.e.,

$$\mu Y_1 + \alpha A^2 + \beta A = \mathcal{E}.$$

These intersections can have very different structures depending on the parameters α, β, and μ of the Hamiltonian and depending on the function $\rho_0(A)$, i.e., on the type of resonance (2.7). One can see that, for every k_+, k_-, there are at most two periodic trajectories corresponding to one energy. When there are two periodic trajectories for some energies $\mathcal{E}$, we call it a "double-well" regime (see Fig. 1), based on the similarities of this case to the well-known problem of the Schrödinger operator $\hat{p}^2 + V(x)$ with a double-well potential $V(x)$ (see [12], [13]).

[2] Nevertheless, the resonance $2:(-1)$ in the Penning trap, where $\mu = 0$, can be analyzed by taking into account the $O(\varepsilon)$-term in (2.13) [11].

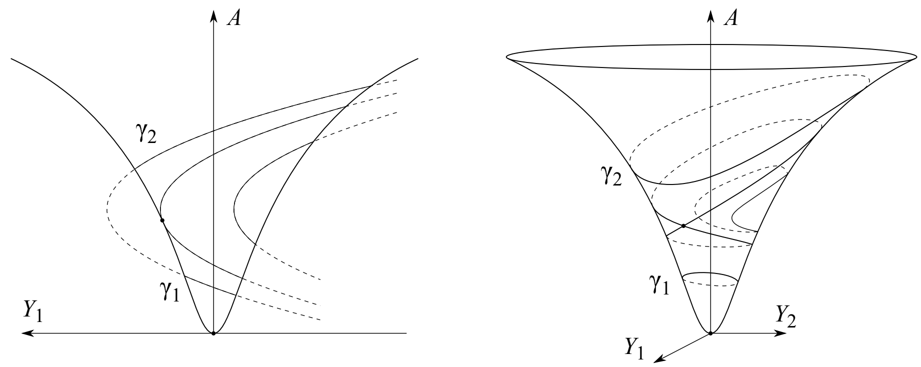

Figure.

Statement 1. *Suppose that the constants α and β have opposite signs $\alpha\beta < 0$. Then, there exists a $\mu_0 > 0$ such that, for any $\mu < \mu_0$, the double-well regime is realized, i.e., there are two periodic classical trajectories corresponding to an energy in some fixed interval.*

If $k_+ + k_- = 4$, then every trajectory is bounded for sufficiently small μ. Otherwise, there is an unbounded classical trajectory for every energy if $k_+ + k_- > 4$. In the double-well regime this unbounded trajectory is separated from the two periodic trajectories by relatively large "barrier"; namely, the width of the barrier in the A-coordinate tends to infinity as $\mu \to 0$.

Proof. The proof is elementary, it based on the analysis of the symplectic leaf surface intersections with the surfaces of constant energy $E = \mathcal{E}$ (see Fig. 1). Let us mention that the polynomial φ_0 takes the form (see (2.12) and (2.9))

$$\varphi_0(a) = (k_- a + 1/\omega_+)^{k_-}(k_+ a)^{k_+}.$$

In the case $\alpha\beta < 0$, the parabola of the energy surface $E = \mathcal{E}$ has its apex in the region $A > 0$. In the limit as $\mu \to 0$, we have two classical trajectories with the constant A, which is a root of the quadratic equation $\alpha A^2 + \beta A = \mathcal{E}$. Thus, there exists a μ_0 such that, for $\mu < \mu_0$, the double-well regime is realized.

A more detailed consideration of the symplectic leaf intersections with the energy surface yields the proof of the remaining part of the statement. □

In Statement 1, the upper bound on μ can be determined as follows. Let us consider the classical trajectories corresponding to the energy $\mathcal{E} = 0$; this energy surface crosses the apex of the symplectic leaf at the origin. We can be sure that the double-well regime is realized if the planes $A = -\beta/2\alpha$ and $A = -2\beta/\alpha$ have empty intersections with the classical trajectories for $\mathcal{E} = 0$. Substituting these values of A into the Hamiltonian and the symplectic leaf (3.3), we obtain the following sufficient conditions for the double-well regime:

$$\mu < \frac{\beta^2}{4|\alpha|}\left(\varphi_0\left(-\frac{\beta}{2\alpha}\right)\right)^{-1/2} \quad \text{and} \quad \mu < \frac{2\beta^2}{|\alpha|}\left(\varphi_0\left(-\frac{2\beta}{\alpha}\right)\right)^{-1/2}. \tag{3.4}$$

Let us mention that, in the case $k_+ + k_- \geq 5$, the unbounded trajectory corresponds to large coordinates A of order $\mu^{-2/(k_+ + k_- - 4)}$, and $Y_{1,2}$ of order $\mu^{-1-4/(k_+ + k_- - 4)}$.

Two distinct implementations of the tunneling effects can appear in our model: first, the tunneling of the state between two periodic bounded trajectories and, second, the tunneling decay of metastable states to infinity.

Remark 1. Actually, conditions (3.4) guarantee the existence of a two-loop separatrix in the whole phase portrait of the Hamiltonian E on the symplectic leaf (3.3). Closed energy curves inside loops represent the double-well regime (see Fig. 1). The hyperbolic equilibrium point on the separatrix represents the top of the barrier between wells.

Let us first consider the tunneling between two periodic trajectories in the double-well regime and omit effects that relate to the unboundedness of the system. This can be done by restricting the operator $\hat{E}$ to a smaller domain of quantum states localized only in the region of $A \in [0, A_0]$, with a large, but fixed, $A_0 > 0$. In the classical framework, it can be realized as an infinite barrier at $A = A_0$. Let us denote the corresponding operator by $\hat{E}_0$. Thus, the spectrum of $\hat{E}_0$ is discrete and the corresponding classical system is bounded.

There are two periodic trajectories $\gamma_{1,2}$ for the energy in the double-well regime (see Fig. 1). The semiclassical quantization rule of classical actions on γ_1 and γ_2 gives two asymptotic series in the discrete spectrum of $\hat{E}_0$. When we change the parameter of the Hamiltonian, the energy levels in these two distinct series change independently, determined by the corresponding classical actions; they form a net-like picture crossing each other (see, for instance, [14], [15]).

The following questions arise:

- Do discrete energy levels of the operator $\hat{E}_0$ have avoided crossings if we continuously change the parameters of the system, or they can cross each other? Is every eigenvalue of $\hat{E}_0$ nondegenerate?
- Can the tunneling energy splitting that appears in the avoided-crossing effect be expressed in terms of complex instantons?
- How does the tunneling rate in the double-well regime between two periodic trajectories relate to the tunneling decay rate of the quantum state in presence of the unbounded trajectories?

All these questions can easily be answered in the framework of the WKB approximation for the Schrödinger operator with the "normal" Hamiltonian $p^2 + V(x)$. Otherwise, for other one-dimensional systems, the answers to these questions can be very different. For instance, in the models describing the large spin of magnetic molecules (see [16], [17]), there appears a degenerate pair of states, and tunneling can be quenched [18], [19].

The success of the tunneling description for the normal one-dimension Schrödinger operator is mostly based on the precise asymptotic estimates of the wave functions in the under-barrier regions, which give the tunneling rate, and on the connection rules, which allow one to construct global asymptotics of wave functions. The absence of such an under—barrier asymptotic of wave functions for arbitrary (pseudodifferential) Hamiltonians makes the study of tunneling in different models an exciting challenge, which has recently attracted much attention (see a survey in [20], [21]).

Let us especially note here the tunneling in the case of the Schrödinger operator with double-well potential and homogeneous magnetic field [22], momentum tunneling for the pendulum Hamiltonian [23]–[25], and tunneling effects for spin Hamiltonians [18], [19], [26]. In all these cases, the calculation was done by applying specially matched unitary transformations, which introduce an effective "tunneling" coordinate. We shall use a similar method below.

4. ACTION-ANGLE DISCRETE REPRESENTATION AND TUNNEL ASYMPTOTICS

In our model, the tunneling effect description, i.e., rigorous answers to all of the above stated questions, can be found by transition to the discrete spectral representation of the action operator $\hat{A}$. The details have been presented in [5], [14].

Statement 2. *If one introduces the action coordinate $q = A$ and the dual coordinate p so that $\hat{p} = -ih\partial_q$, then the irreducible representation of the algebra* (2.11) *with $\hat{K} = 0$ can be realized by*

$$\hat{A} = \hat{q}, \qquad \hat{B} = b_h(\hat{q})e^{-i\hat{p}}. \tag{4.1}$$

This operator representation is determined in the space $\ell^2(X)$ of square-summable sequences over the discrete set $X = \{0, h, 2h, \dots\}$ where the coordinate q takes values. Here $b_h(q) \overset{def}{=} \sqrt{\varphi_h(q)}$, $b_h(q) > 0$ for $q \in X$, $q \neq 0$, and $b_h(0) = 0$.

The spectral problem for the operator $\hat{E}$ takes the form of the following second-order h-difference equation

$$\frac{\mu}{2}b_h(q+h)\,y(q+h)+\frac{\mu}{2}b_h(q)\,y(q-h)+(\alpha q^2+\beta q)\,y(q)=\mathcal{E}\,y(q), \tag{4.2}$$

where $y(q)\in\ell^2(X)$ and $\mathcal{E}$ is a spectral parameter. The operator $\hat{E}_0$ corresponds to Eq. (4.2) with the additional Dirichlet boundary condition $y(q)=0$, $q>A_0$.

The coordinates (q,p) can be understood as local Darboux coordinates on the symplectic leaf (3.3) of the Poisson algebra (3.2)

$$A=q,\qquad Y_1=b_0(q)\cos(p),\qquad Y_2=b_0(q)\sin(p).$$

Thus, the coordinate p is just the "angle" dual to the "action" coordinate A. In these coordinates, the Hamiltonian $\hat{E}$ and the difference equation (4.2) can be recognized as a generalized pendulum system.

The properties of second-order difference equations are very similar to those of second-order differential equations [27], [28].

Statement 3. *The spectrum of $\hat{E}_0$ is discrete and nondegenerate. If the parameters of the Hamiltonian in the double-well regime are continuously changed, the different eigenvalues of $\hat{E}_0$ do not cross each other, but have avoided-crossings.*

Near the avoided-crossing values of parameters, the corresponding eigenstates of $\hat{E}_0$ are bilocalized on the symplectic leaf (3.3) *in both phase space wells surrounded by periodic classical trajectories (see Statement 1). These states form a semiclassical bi-state in the sense of* [5].

In order to formulate some results on under-barrier (tunneling) semiclassical asymptotics of difference equation solutions, we need to fix the following notation. Let us introduce the classical Hamiltonian E in (q,p) coordinates by the Weyl symmetrized symbol (see [29])

$$E_h(q,p)=\mu b_h(q+h/2)\cos(p)+\alpha q^2+\beta q. \tag{4.3}$$

The Hamiltonian $E_h(q,p)$ is a 2π-periodic function of the momentum p, and the classical phase space is a half-cylinder with $q>-h/2.$, i.e., we identify all phase space points with momenta that differ by 2π. The equation $E_h(q,p)=\mathcal{E}$ defines two smooth branches of $p=\pm p_h(q,\mathcal{E})$ (mod 2π). The branch points of p are the turning points of the corresponding classical system (points where the classical velocity $v(q,\mathcal{E})=\partial_p E_0(q,p)|_{p=p_0(q,\mathcal{E})}$ vanishes), which satisfy the equation

$$\pm\mu b_h(q+h/2)+\alpha q^2+\beta q=\mathcal{E},$$

where the signs "+" and "−" correspond to the turning points with $p=0$ and $p=\pi$, respectively.

Lemma 1. *On any interval $[q_1,q_2]$ without turning points, Eq.* (4.2) *has two linearly independent solutions of the form*

$$y_\pm(q,h)=\frac{1}{\sqrt{v(q,\mathcal{E})}}\exp\biggl(\pm\frac{i}{h}\int_{q_1}^{q}p_h(q,\mathcal{E})\,dq\biggr)[1+O(h)]. \tag{4.4}$$

The asymptotic estimate is uniform for $q\in[q_1,q_2]\cap X$.

The rigorous proof of the discrete WKB approximation (4.4) can be done by methods from [30]; see details in [29] and also see [26], [31]–[33] on the theory and application of the discrete WKB.

One can see that the asymptotics (4.4) are identical in form to those of the continuous WKB approximation to the Schrödinger equation. The significant difference appears in the dependence of momentum p on the coordinate q. For instance, in the classically forbidden region, $Re\,p$ is constant; namely, $Re\,p=0$ or $Re\,p=\pi$ depending on the types of corresponding turning points. Thus, the normalized wave functions exponentially decrease under the barrier as $h\to 0$, and (4.4) gives the corresponding tunneling rate.

5. SPECTRAL SPLITTING AND PERIODIC INSTANTONS

Suppose the parameters of the system are chosen in such a way that the "double-well" regime is realized (Statement 1). Then, for a given energy $\mathcal{E}$, there are two periodic classical trajectories $\gamma_{1,2}$ and also one unbounded trajectory γ_∞ in the case $k_+ + k_- \geq 5$.

Let ψ_1 and ψ_2 be the normalized approximate stationary states of $\hat{E}$ that are localized near the periodic trajectory γ_1 and γ_2, respectively. They can be rigorously defined as solutions of the difference equation (4.2) with additional Dirichlet boundary conditions on points under the classical barriers.

Under variation of the parameters in the avoided-crossing effect two energy levels of the operator $\hat{E}_0$ approach each other to a minimum distance Δ and then repel, while the corresponding precise stationary states form a linear combinations of the localized states ψ_1 and ψ_2. The minimal splitting Δ is exponentially small as $h \to 0$:

$$\Delta = \exp\biggl(-\frac{\mathcal{S}}{h}(1 + o(1))\biggr). \tag{5.1}$$

It is well known that the description of the tunneling dynamics of a quantum particle in the semiclassical approximation is closely related to the complexification of classical Hamiltonian equations [23], [34], [35].

Let us consider the complexification of the Poisson algebra (2.11), symplectic leaf (3.3), Hamiltonian E and the corresponding trajectories of motion taking pure imaginary time $t = -i\tau$. We say that the periodic complex trajectory $\tilde{\gamma}$ is an *instanton* if it corresponds to the energy $\mathcal{E}$ and crosses two real classical trajectories (see [14], [36]).

In the case $k_+ + k_- \geq 5$, there are two instantons $\tilde{\gamma}_{1,2}$ for a given energy in the double-well regime. The instanton $\tilde{\gamma}_1$ connects two periodic trajectories γ_1 and γ_2, it corresponds to the avoided-crossing effect in the spectrum of $\hat{E}_0$. The other instanton $\tilde{\gamma}_2$ relates to the classical barrier between γ_2 and γ_∞, and it corresponds to the tunneling decay of metastable states of $\hat{E}$.

Theorem 1. *The avoided-crossing energy splitting for the pendulum Hamiltonian $\hat{E}_0$ has the form* (5.1)*, where the corresponding tunneling action $\mathcal{S}$ is the action on the instanton $\tilde{\gamma}_1$*:

$$\mathcal{S} = \frac{1}{2i}\int_{\tilde{\Sigma}_1} dp \wedge dq > 0. \tag{5.2}$$

Here the surface $\tilde{\Sigma}_1$ is spanned by the instanton $\tilde{\gamma}_1$, i.e., $\partial\tilde{\Sigma}_1 = \tilde{\gamma}_1$.

The tunneling decay rate of metastable states of the operator $\hat{E}$ is exponentially small with the exponent determined by the tunneling action $\mathcal{S}_2$ of the form

$$\mathcal{S}_2 = \frac{1}{2i}\int_{\tilde{\Sigma}_2} dp \wedge dq > 0, \tag{5.3}$$

where the surface $\tilde{\Sigma}_2$ is spanned by the instanton $\tilde{\gamma}_2$.

Proof. The derivation of formulas (5.2) and (5.3) is similar to that presented in [14]. It is based on the under-barrier asymptotic of the wave functions (see Lemma 1).

Let the parameters of the Hamiltonian be tuned so that the minimal energy splitting Δ is realized in the avoided-crossing effect for the operator $\hat{E}_0$, and let $\psi_{I,II}$ be the corresponding bilocalized eigenstates. Therefore, these normalized states have the form $\psi_{I,II} = (\psi_1 \pm \psi_2)/\sqrt{2}$ up to exponentially small corrections as $h \to 0$.

Using Lemma 1, we see that the states $\psi_{1,2}$ have the following asymptotic estimates in the under-barrier region of q between γ_1 and γ_2:

$$\psi_1(q,h) = \frac{c_1}{\sqrt{v(q,\mathcal{E})}}\exp\biggl(\frac{i}{h}\int_{q_1}^{q} p_h(q,\mathcal{E})\,dq\biggr)[1 + O(h)],$$

$$\psi_2(q,h) = \frac{c_2}{\sqrt{v(q,\mathcal{E})}}\exp\biggl(\frac{i}{h}\int_{q}^{q_2} p_h(q,\mathcal{E})\,dq\biggr)[1 + O(h)],$$

where $q_{1,2}$ are turning points, and we take the branch of the momentum $p = p_h(q, \mathcal{E})$ for which $Im\, p > 0$, i.e., the states $\psi_{1,2}$ exponentially decrease (in absolute value) in the under-barrier region as $h \to 0$. It can be shown that the normalizing constants $c_{1,2}$ have the order of $\exp(o(1/h))$, i.e., they cannot change the leading term of the exponent phase.

The further derivation of the tunneling estimates (5.1), (5.2), (5.3) is similar to the case of the well-known case of the Schrödinger equation (see [13]). □

Estimating two tunneling actions $\mathcal{S}$ and $\mathcal{S}_2$, one can see that the tunneling action $\mathcal{S}_2$ is much larger than the action $\mathcal{S}$ for sufficiently small μ; namely,

$$\frac{\mathcal{S}}{\mathcal{S}_2} = O(\mu^{2/(k_+ + k_- - 4)}) = O(\varepsilon). \tag{5.4}$$

Therefore, we can conclude that the tunneling between two periodic trajectories in our model is more significant than the tunneling decay of the quantum state. This is an example of semiclassical bistates and 2-level subsystems discussed in [5].

Remark 2. The geometric description of the double-well regime stated above and the corresponding tunneling effects are stable under the inclusion of higher-order terms from (2.2), (2.5) to the averaging procedure. These terms give only small (of order ε) corrections to the periodic classical trajectories, to the instanton $\tilde{\gamma}_1$ and the corresponding tunneling action $\mathcal{S}$.

Corollary 1. *The existence of avoided crossings, the state bilocalization, the spectral splitting and its geometric description, as in Theorem 1, take place for the whole trap Hamiltonian* $\mathbb{H}$ (2.1)*,* (2.2).

Let us focus on the resonance $3 : (-1)$ as in (2.14). In this case, it is possible to extend the above statements to nonpolynomial Hamiltonians (as in the Penning trap situation [5]). The point is that very high anharmonic terms in the expansion like (2.2) can be made negligible by choosing ε to be exponentially small with respect to h.

The exponential smallness of $\varepsilon = \hbar\omega(n)$, in turn, is provided by choosing not very large values of the trap energy $\omega(n)$. Indeed if $\omega(n) = c\ln(1/\hbar)$ then $\varepsilon \leq c\exp(-d/h)$ with $d = (e-1)/ec > 0$.

Note that, in the usual "quasi-classical" approximation zone, one deals with low energy levels of value $\omega(n) \sim 1$. In this zone, $\varepsilon \sim \hbar$, but the effective Planck constant in (2.6) is not small: $h \sim 1$. Thus, on quasi-classical energy levels, the trap becomes purely quantum and one cannot relate the tunneling bilocalization of its states to any symplectic geometry or instantons as in (5.1)–(5.3).

On the contrary, in the "semiclassical" zone where $\omega(n) \sim 1/\hbar$ the effective Planck constant $h \sim \hbar$ is small. But, in this zone, the parameter $\varepsilon \sim 1$ becomes not small and one cannot apply perturbation theory to higher-order anharmonic terms in (2.5).

In the "mezzo-classical" zone $\omega(n) \sim \ln(1/\hbar)$, the effective Planck constant $h \sim 1/\ln(1/\hbar)$ is small enough and the parameter ε is exponentially small with respect to h.

Theorem 2. *Take* $N = \infty$ *in* (2.2)*, i.e., let the Hamiltonian be a nonpolynomial. Suppose a resonance* $3 : (-1)$ *takes place for frequencies of* H_0 (2.3) *and the parameters of the effective Hamiltonian* (3.1) *are taken in the "double-well" regime (as in Statement 1).*

Then, under condition $\ln(1/\hbar) \gg 1$*, in the mezzo-classical zone, i.e., for not very excited energy levels of the operator* $\mathbb{H}$*, namely, for eigenvalues of the order of* $\ln(1/\hbar)$*, there is an avoided-crossing energy splitting with asymptotics* (5.1) *determined by the instanton action* (5.2)*, as well as the bilocalization effect of the corresponding eigenstates*[3].

[3]Note that if the original trap Hamiltonian describes an unbounded system and the corresponding operator has a continuous spectrum, then the bilocalized states are not eigenstates of the trap Hamiltonian, but are long-living metastable states.

Proof. Under assumptions of the theorem, the unitary averaging operator U identifies the trap Hamiltonian $\mathbb{H}$ with model Hamiltonian $\hat{E}$, i.e., $\mathbb{H} = U\hat{E}U^{-1}$, up to a correction of order ε^m for some fixed m. In the mezzo-classical zone, the correction is exponentially small as $h \to 0$ and by choosing m, we can make it exponentially smaller than Δ.

Let $\psi_{I,II}$ be a pair of bilocalized eigenstates of the operator $\hat{E}$, as in Theorem 1. Then $\Psi_{I,II} = U\psi_{I,II}$ is a pair of bilocalized metastable states of the trap operator, i.e., they obey the spectral equation of the operator $\mathbb{H}$ with small discrepancy. The key point here is that the corresponding exponentially small energy splitting Δ is much greater than that discrepancy. If the trap is stable and the corresponding spectrum of $\mathbb{H}$ is discrete, then there appears a pair of bilocalized states of the trap. Otherwise, the $\Psi_{I,II}$ are long-living metastable states of the trap and the living time of $\Psi_{I,II}$ is much greater than the tunneling time $2\pi h/\Delta$. □

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