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Bi-States and 2-Level Systems in Rectangular Penning Traps

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Abstract. We introduce a notion of semiclassical bi-states. They arise from pairs of eigenstates corresponding to tunnel-splitted eigenlevels and generate 2-level subsystems in a given quantum system. As an example, we consider the planar Penning trap with rectangular electrodes assuming the $3 : (-1)$ resonance regime of charge dynamics. We demonstrate that, under small deviation of the rectangular shape of electrodes from the square shape (symmetry breaking), there appear instanton pseudoparticles, semiclassical bi-states, and 2-level subsystems in such a quantum trap.

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1. INTRODUCTION

Beginning from Feynman's paper [1], the quantum computations are related to open 2-level systems. A more recent notion from quantum informatics, a q-bit, is sometimes simply identified with the notion of 2-level system [2]. The opportunity to generate mixed and entangled states in such systems makes them very interesting for studying from the viewpoint of algebra, geometry, and functional analysis.

For recognition of suitable 2-level subsystems in a given quantum system, one has to check the following basic properties:

(i) there are two distinguished eigenstates ψ_1, ψ_2 of the system corresponding to close to each other eigenvalues $\lambda_1 < \lambda_2$ and the gap $\lambda_2 - \lambda_1$ is much less than the distance from λ_1 and λ_2 to the rest spectrum of the system;

(ii) a generic external observable mixes the states ψ_1 and ψ_2, i.e., its matrix in the basis ψ_1, ψ_2 is not diagonal (with a certain accuracy);

(iii) the probability of transition from the level λ_1 to lower energy levels of the whole system is small enough.

In this paper, we first of all discuss how the 2-level subsystems can be generated via the tunnelling bi-localization effect in the semiclassical framework. And secondly, we demonstrate that such tunnel 2-level subsystems appear in trapping systems at frequency resonance which makes the algebra of integrals of motion to be noncommutative and under symmetry breaking which creates pseudoparticles (instantons) over this noncommutative algebra.

Our main example of trapping system is a planar rectangular Penning trap with $3 : (-1)$ resonance between the modified cyclotron and magnetron frequencies. We demonstrate that the periodic instanton regime and 2-level system in the space of integrals of motion originate in the trap geometric asymmetry (a deviation of rectangle electrodes from square shape).

Under suitable fine co-tuning of electric voltage and magnetic field strength such a 2-level system even could depend on a continuous free parameter.

2. SEMICLASSICAL BI-STATES

For simplicity, assume that we deal with the simplest model of a quantum system realized by the Hilbert space $\mathcal{L} = L^2(\mathbb{R})$ and by the algebra of Weyl-symmetrized observables $\hat{f} = f(\hat{q}, \hat{p})$, $\hat{p} = -ih\partial/\partial q$, $q \in \mathbb{R}$ [3]. Denote by the asterisk $*$ the Groenewold–Moyal product in this algebra: $\hat{f}\hat{g} = \widehat{f * g}$.

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For any pair of wave functions $\psi_1, \psi_2 \in \mathcal{L}$, we introduce a density 2-matrix $D = ((D_{jk}))$, $j, k = 1, 2$. Each element D_{jk} is a linear functional determined on phase space functions as follows

$$D_{jk}(f) \stackrel{\text{def}}{=} (\hat{f}\psi_j, \psi_j), \qquad f \in C_0^\infty(\mathbb{R}^2).$$

The parentheses on the right-hand side denote the scalar product in $\mathcal{L}$.

One can represent the density 2-matrix as a quaternion

$$D = \sum_{\alpha=0}^{3} d_\alpha \sigma_\alpha, \quad \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.1}$$

The functionals d_α satisfy the inequality

$$d_0(f)^2 \geqslant d_1(f)^2 + d_2(f)^2 + d_3(f)^2$$

on the subspace of observables $f = g * \bar{g}$. This is an analog of the known condition on the Stokes parameters of quasimonochromatic radiation.

Let $\hat{H}$ be the Hamiltonian of the system in consideration.

Definition 2.1. A *semiclassical bi-state* is a pair of eigenstates ψ_1, ψ_2 corresponding to different but h^∞-close eigenvalues of $\hat{H}$ such that their density 2-matrix is not diagonal up to $O(h^\infty)$ in the weak sense (as a linear functional).

The last condition on the density 2-matrix means that the cross mean value $(\hat{f}\psi_1, \psi_2)$ is not a quantity of order $O(h^\infty)$ for a generic observable f. This implies the key property (ii) of the 2-level subsystem discussed in the Introduction.

Example 2.1. For the Schrödinger operator with a single-well (unique equilibrium point) potential, there are no semiclassical bi-states.

Example 2.2. If the oscillation supports [3] of ψ_1 and ψ_2 do not intersect, $\mathrm{osc}_\infty(\psi_1) \cap \mathrm{osc}_\infty(\psi_2) = \emptyset$, then the pair ψ_1, ψ_2 is not a semiclassical bi-state. Thus, for the Schrödinger operator with a double-well potential, if the eigenstates ψ_1 and ψ_2 are asymptotically (as $h \to 0$) localized in different wells, then they do not form a semiclassical bi-state.

Example 2.3. It is known that the generic distance between eigenvalues of the Schrödinger operator $\hat{H} = \hat{p}^2 + V(\hat{q})$ is of order h. But in the case of a double-well potential V some pairs of eigenvalues, say λ_1, λ_2, may be displaced at an exponentially small distance as $h \to 0$ due to the tunnelling effect. The corresponding pairs of eigenstates ψ_1, ψ_2 are bi-localized in both wells [4].

In this situation, there exist wave functions φ_I, φ_{II} which are

– asymptotically localized in different wells of the potential,

– approximately satisfy the Schrödinger equation $\hat{H}\varphi_j = \lambda_j \varphi_j + O(h^\infty)$ $(j = I, II)$,

– their linear combinations asymptotically represent the exact eigenfunctions ψ_1, ψ_2 as

$$\psi_1 = g\varphi_I + \sqrt{1-g^2}\varphi_{II}, \qquad \psi_2 = \sqrt{1-g^2}\,\varphi_I - g\varphi_{II} \pmod{h^\infty} \tag{2.2}$$

for some $0 < g < 1$, for details see, e.g., [5]. Thus, if we denote the Wigner function corresponding to φ_j by ρ_j, then $\bmod h^\infty$ we obtain in (2.1)

$$d_0 = \frac{1}{2}(\rho_I + \rho_{II}), \quad d_1 = g\sqrt{1-g^2}(\rho_I - \rho_{II}), \quad d_2 = 0, \quad d_3 = (g^2 - \frac{1}{2})(\rho_I - \rho_{II}).$$

Since $\mathrm{osc}_\infty(\varphi_I) \cap \mathrm{osc}_\infty(\varphi_{II}) = \emptyset$, the supports of ρ_I and ρ_{II} $\bmod h^\infty$ do not intersect, and therefore the density 2-matrix D is not diagonal $\bmod h^\infty$. Thus the pair ψ_1, ψ_2 is a semiclassical bi-state.

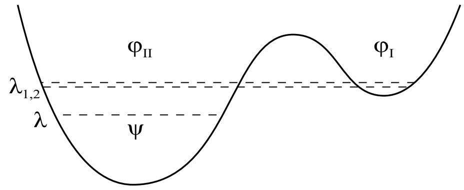

Fig. 1

Proposition 2.1. *Any bilocalized pair of states corresponding to tunnel-splitted eigenlevels generates a semiclassical bi-state and satisfies properties* (i), (ii) *for* 2*-level subsystem.*

Now assume that the double-well potential has a specific shape as in Fig. 1 and the bilocalized states ψ_1, ψ_2 correspond to energy levels $\lambda_1 < \lambda_2$ which are the lowest for the right well. Assume that the wave function φ_I in representation (2.2) is localized in the right well, and φ_{II} is localized in the left one.

Let us consider an eigenlevel λ of $\hat{H}$ which lies under the bottom of the right well and denote the eigenstate of $\hat{H}$ corresponding to λ by ψ. The probability $\mathrm{pr}(\psi_1 \to \psi)$ of transition from ψ_1 to ψ is estimated as the matrix element

$$\begin{aligned}\mathrm{pr}(\psi_1 \to \psi) \sim (\hat{q}\psi_1, \psi) &= g(\hat{q}\varphi_I, \psi) + \sqrt{1-g^2}(\hat{q}\varphi_{II}, \psi) + O(h^\infty) \\ &= \sqrt{1-g^2}(\hat{q}\varphi_{II}, \psi) + O(h^\infty).\end{aligned}$$

Here we used representation (2.2) and the fact that $\mathrm{osc}_\infty(\varphi_I) \cap \mathrm{osc}_\infty(\psi) = \emptyset$.

Proposition 2.2. *The probability* $\mathrm{pr}(\psi_1 \to \psi)$ *will be small enough if the coefficient* g *in representation* (2.2) *is chosen closer to* 1, *i.e., if the lowest eigenfunction* ψ_1 *is localized in the right well more than in the left one. Then the bi-state* ψ_1, ψ_2 *will possess property* (iii) *of* 2*-level subsystem.*

Note that if the double-well potential V depends on an external parameter, then by suitable tuning of this parameter one can reach the tunnel bi-localization effect on the lowest levels λ_1, λ_2 for the right well and also control the coefficient g in (2.2) to obtain the desirable 2-level subsystem with the whole bunch of properties (i)–(iii).

3. RECTANGULAR PENNING TRAP UNDER 3 : (−1) RESONANCE

As a model for above mathematical notions let us consider an asymmetric version of the usual [6, 7] planar Penning trap holding an electron. Let the system of the trap electrodes be displaced on a plane and consists of

(1) the internal rectangle electrode with sizes $2a_1 \times 2a_2$; its half-diagonal is $|a| = \sqrt{a_1^2 + a_2^2}$, and the asymmetry parameter is $T \stackrel{\text{def}}{=} (a_2/a_1)^2 \leqslant 1$;

(2) the ring-shape rectangular electrode surrounding the internal one and having outer sizes $2\varkappa a_1 \times 2\varkappa a_2$, where $\varkappa \gg 1$ is a large parameter which determines the effective spatial scale $l_\varkappa \stackrel{def}{=} |a|/\varkappa$ of the charge dynamics;

(3) the third external electrode which is just the rest (infinite) part of the plane.

Another key feature of the trap is a homogeneous magnetic field B directed perpendicularly to the plane of the electrodes. It determines a scale for electric voltage: $V_0 \stackrel{\text{def}}{=} eB^2|a|^2/mc^2$, as well as the Bohr magneton energy scale $\lambda_B = \hbar eB/mc$ and the Lorentz length scale $l_\perp \stackrel{\text{def}}{=} \sqrt{e/B}$.

Stability of the charge dynamics along the magnetic axis is ensured by the electric field created by the system of electrodes. We assume that on the infinite third electrode one keeps the voltage 0, to the second ring-shaped electrode apply the voltage $-\varkappa v$ (in V_0-units), and to the first rectangle electrode apply the voltage $(-\varkappa + d)v$. Here $v > 0$ and $3/2 < d < 5/2$ are dimensionless parameters; the relation $v = v_T(d)$ between them and the asymmetry parameter T will be set below in (3.10) in order to reach a resonance of the trap frequencies.

Let us denote by U the electric potential (in V_0-units) obtained by solving the Laplace equation $\Delta U = 0$ with the described boundary conditions on the trap electrodes. The function U has a saddle point on the trap axis directed along the magnetic field and starting from the center of electrodes. The distance $\xi = \xi_T(d)$ of this point from the plane of electrodes is determined (in $|a|$-units) by solving the equation

$$\frac{\sqrt{1+\xi^2}(1+(1+T)\xi^2)(1+(1+1/T)\xi^2)}{(1+2\xi^2)} = d. \tag{3.1}$$

The harmonic (quadratic) part U_0 of the potential U near the saddle point has the signature $(-,-,+)$ with plus $+$ along the trap axis. The second derivatives at the saddle point are given by $(-\omega_1^2, -\omega_2^2, \omega_0^2)$, where $\omega_0^2 = \omega_1^2 + \omega_2^2$ and

$$\begin{aligned} \omega_1^2 &= \frac{2vd\sqrt{T}\,\xi\left(3+2T+3(1+T)\xi^2\right)}{\pi\left(1+\xi^2\right)^{3/2}\left(1+(1+T)\xi^2\right)^2}, \\ \omega_2^2 &= \frac{2vd\sqrt{T}\,\xi\left(2+3T+3(1+T)\xi^2\right)}{\pi\left(1+\xi^2\right)^{3/2}\left(T+(1+T)\xi^2\right)^2}. \end{aligned} \tag{3.2}$$

Note that in (3.1), (3.2) we omit the corrections of order $1/\varkappa^2$ which can be taken into account by perturbation theory later on.

Denote by u_0 the value of U_0 at the saddle point. Then the Hamiltonian of the trap (in λ_B/h-units) on the energy levels around $\varkappa^2 u_0$ can be represented as

$$\hat{H} = \varkappa^2 u_0 + \hat{H}_0 + \frac{1}{\varkappa}\hat{U}_1 + \frac{1}{\varkappa^2}\hat{U}_2 + O\left(\varkappa^{-3}\right). \tag{3.3}$$

Here the quantization hat-sign, as in Sect. 2, means the correspondence $q \to \hat{q}$, $p \to \hat{p} = -ih\partial_q$, where q are the Euclidean coordinates (in $l_\varkappa$-units) with the origin at the saddle point. The parameter $h \overset{\text{def}}{=} \frac{1}{\alpha}(l_\perp/l_\varkappa)^2$ is the effective "Plank constant" where $\alpha = e^2/\hbar c \approx 1/137$ is the fine structure constant. The regime $h \ll 1$ of semiclassical approximation, which we assume below, takes place iff

$$(l_\perp/l_\varkappa)^2 \ll \alpha \qquad \text{or} \qquad \varkappa \ll \sqrt{\alpha}\,|a|/l_\perp. \tag{3.4}$$

By U_1 and U_2 in (3.3) we denoted the components of the electric potential U which are polynomials of degree 3 and 4 in spatial coordinates q. The leading term H_0 in (3.3) is the ideal Penning trap Hamiltonian:

$$H_0 = \frac{1}{2}(p + \mathcal{A}(q))^2 + U_0(q), \tag{3.5}$$

the vector-potential $\mathcal{A}$ corresponds to the unit homogeneous magnetic field directed along the trap axes.

The Hamiltonian H_0 (3.5) can be represented in normal form with three normal frequencies ω_+, $(-\omega_-)$, $\omega_0 = \sqrt{1-\omega_+^2-\omega_-^2}$ which are calculated by known formulas [6].

In the symmetric case $a_1 = a_2$ (square shape) one has $\omega_1 = \omega_2$ and the normal frequencies obey

$$\omega_+ + \omega_- = 1, \quad \omega_0 = \sqrt{2\omega_+\omega_-}. \tag{3.6}$$

The normal form of the Hamiltonian $\hat{H}_0$ reads

$$\hat{H}_0 = \omega_+\hat{S}_+ - \omega_-\hat{S}_- + \omega_0\hat{S}_0 + h\left(\omega_+ - \omega_- + \omega_0\right)/2, \tag{3.7}$$

where $\hat{S}_j$ are the mutually commuting action operators with equidistant spectra

$$\operatorname{Spec}(\hat{S}_j) = \{n_j h \mid n_j = 0, 1, 2, \dots\}, \quad j \in \{+, -, 0\}. \tag{3.8}$$

This simplest type of Hamiltonians do not obey any bi-state and 2-level subsystems. And moreover, if the frequencies in (3.7) are not in resonance then the whole Hamiltonian $\hat{H}$ (3.3) also does not admit such structures since after a unitary (averaging) transformation it is reduced with accuracy $O(\varkappa^{-\infty})$ to some function in action operators.

Therefore, we have to analyze a resonance regime, which provides an opportunity to obtain (after averaging) a nontrivial Hamiltonian with creation–annihilation structure generating bi-states and 2-level systems.

The basic non degenerate resonance $\omega_+ : (-\omega_-) = 2 : (-1)$, as well the next one $3 : (-1)$, were investigated in [8, 9]. The creation–annihilation regime appeared due to the symmetry breaking. In [8] we used the perturbing inhomogeneous magnetic Ioffe field and in [9] — used a small inclination of the magnetic field from the trap axis.

In the present work we study the resonance $3 : (-1)$ between normal frequencies ω_+ and $(-\omega_-)$ without any deformation of the homogeneous magnetic field but with asymmetry in the geometry of the trap electrodes. The asymmetry, i.e., the deviation of T from 1, can be small or not small at all; in particular, we do not relate the value of asymmetry with the perturbing small parameter $1/\varkappa$ in Hamiltonian (3.3).

In the asymmetric case relations (3.6) do not hold, but still $\omega_+^2 + \omega_-^2 + \omega_0^2 = 1$. Thus assuming a resonance regime $3 : (-1) : t$ with some unknown t we obtain the relations

$$\omega_+^2 = \frac{3^2}{3^2 + 1^2 + t^2} = \frac{9}{10 + t^2}, \qquad \omega_-^2 = \frac{1}{3^2 + 1^2 + t^2} = \frac{1}{10 + t^2}. \tag{3.9}$$

From these two equations we determine the value of the parameter $v = v_T(d)$ in (3.2) and the value of the number $t = t_T(d)$ from the resonance proportion. Of course, in the symmetric case $T = 1$ the value of t can be derived from (3.6), which gives $t = t_1(d) \equiv \sqrt{6}$ for any d. The explicit formula for v up to $1/\varkappa^2$ reads

$$v_T(d) = 3\sqrt{T}\pi(1 + \xi^2)(1 + (1 + T)\xi^2)(T + (1 + T)\xi^2)(1 + 2\xi^2)/[2\xi(10\gamma + 3(1 + T)\beta)], \tag{3.10}$$

where

$$\gamma = (1 + (1 + T)\xi^2)(T + (1 + T)\xi^2)\sqrt{(3 + 2T + 3(1 + T)\xi^2)(2 + 3T + 3(1 + T)\xi^2)},$$
$$\beta = 2 + T + 2T^2 + (7 + 12T + 7T^2)\xi^2 + 11(1 + T)^2\xi^4 + 6(1 + T)^2\xi^6,$$

and $\xi = \xi_T(d)$ is the solution of (3.1).

Proposition 3.1. *Under the choice $v = v_T(d) + O(1/\varkappa^2)$, where $v_T(d)$ is given by (3.10), the Hamiltonian $\hat{H}_0$ of the ideal Penning trap possesses the $3 : (-1)$ resonance between modified cyclotron frequency ω_+ and magnetron frequency ω_- for any $d \in [\frac{3}{2}, \frac{5}{2}]$ and $T \in [\frac{1}{2}, 1]$.*

Due to the resonance between ω_+ and ω_- in (3.7) the Hamiltonian $\hat{H}_0$ has a noncommutative algebra of integrals of motion, i.e., operators commuting with $\hat{H}_0$ (see in [10]). This algebra is generated by three actions $\hat{S}_+$, $\hat{S}_-$, $\hat{S}_0$ and the pair of creation–annihilation operators $\hat{B}$, $\hat{B}^*$. Commutation relations between these generators are nonlinear (non-Lie); for details, see [8]:

$$\begin{aligned} &[\hat{B}^*, \hat{B}] = h\Big(\hat{S}_+\hat{S}_-^2 + \frac{1}{9}\hat{S}_-^3 + h\Big(\hat{S}_+\hat{S}_- + \frac{2}{3}\hat{S}_-^2\Big) + \frac{h^2}{9}(6\hat{S}_+ + 11\hat{S}_-) + \frac{2h^3}{3}\Big), \\ &[\hat{S}_+, \hat{B}] = h\hat{B}, \qquad [\hat{S}_-, \hat{B}] = 3h\hat{B}. \end{aligned} \tag{3.11}$$

This algebra has Casimir elements

$$\hat{S}_0, \quad \hat{C} = 3\hat{S}_+ - \hat{S}_-, \quad \text{and} \quad \hat{K} = \hat{B}\hat{B}^* - \frac{1}{9}\hat{S}_+\hat{S}_-(\hat{S}_- - h)(\hat{S}_- - 2h). \tag{3.12}$$

In the discussed model, we deal with irreducible representations of this algebra, where the operator $\hat{K} = 0$.

By using the operator averaging procedure [8], one can unitarily transform the Hamiltonian (3.3) to the commutative form

$$\hat{H} \sim \varkappa^2 u_0 + \hat{H}_0 + \frac{1}{\varkappa^2}\hat{H}_2 + O\Big(\frac{1}{\varkappa^3}\Big), \tag{3.13}$$

where the correction $\hat{H}_2$ commutes with $\hat{H}_0$ and thus can be represented as a polynomial in generators of algebra (3.11). The formula for $\hat{H}_2$ reads

$$\hat{H}_2 = \eta(\hat{B} + \hat{B}^*) + \frac{1}{2}\sum_{j,k}\eta_{jk}\hat{S}_j\hat{S}_k + \sum_j \eta_j\hat{S}_j + \zeta. \tag{3.14}$$

The explicit expressions for the coefficients in (3.14) are cumbersome; we write down their asymptotics in the Appendix near the quadratic-shape breaking value, i.e., assuming that $T = 1-\varepsilon$, where $\varepsilon \ll 1$.

For simplicity, we below consider the energy levels of $\hat{H}$ closest to $\varkappa^2 u_0$ by choosing only those representations of algebra (3.11) where the values of Casimir elements $\hat{S}_0$ and $\hat{C}$ are of order h, i.e., choose the quantum numbers n_0 and $n_c \equiv 3n_+ - n_-$ in (3.8) to be of order 1.

Proposition 3.2. *In 3 : (−1) resonance regime, by a unitary transform the trap Hamiltonian can be written in the form* (3.13)*, where* $[\hat{H}_0, \hat{H}_2] = 0$. *On energy levels closest to* $\varkappa^2 u_0$ *the anharmonic part of the Hamiltonian has the following form*

$$\hat{H}_2 = \mu(\hat{E} + c), \qquad \hat{E} = \varepsilon(\hat{B} + \hat{B}^*) + a\hat{S}_+^2 + b\hat{S}_+, \tag{3.15}$$

where $\hat{B}$ *are the generators of the algebra* (3.11)*. There are two free parameters in this representation: the parameter* d *determining the difference of voltages on trap electrodes and a parameter* k *in possible perturbation of the magnetic field value* $B(1 + k/\varkappa^2)$*. The dependence of coefficients* μ*,* a*,* b*, and* c *in* (3.15) *from* d *is explicitly shown in the Appendix. The second perturbing parameter* k*, when it is taken to be nonzero, will be presented only in the coefficients* b *and* c *(in an additional summands proportional to* k *with numerical multipliers).*

4. DIFFERENCE OPERATOR REPRESENTATION AND SEMICLASSICAL QUANTIZATION RULE

Thus the model of the planar resonance Penning trap is reduced to the top-like Hamiltonian (3.15) over the non-Lie algebra (3.11) with known numerical coefficients depending on two free parameters.

We shall realize the irreducible representations of the algebra (3.11) by using the spectral representation of the operator $\hat{S}_+$ and the difference operator representation of $\hat{B}$.

Proposition 4.1. *If one introduces the coordinate operator* $\hat{q} = \hat{S}_+$ *and the momentum* $\hat{p} = -ih\partial_q$ *then the irreducible representation of the algebra* (3.11) *with* $\hat{C} = hn_c$ *and* $\hat{K} = 0$ *takes the form*

$$\begin{aligned} &\hat{S}_+ = \hat{q}, \qquad \hat{S}_- = 3\hat{q} - hn_c, \\ &\hat{B} = \beta(\hat{q}, h)e^{-i\hat{p}}, \qquad \beta(q,h) = \frac{1}{3}\sqrt{q(3q - hn_c)(3q - hn_c - h)(3q - hn_c - 2h)}. \end{aligned} \tag{4.1}$$

In view of (3.8) *the coordinate* $\hat{q}$ *takes the discrete values in* $X = \{q_0, q_0 + h, q_0 + 2h, \dots\}$*, where*

$$q_0 = \begin{cases} 0, & n_c \leqslant 0; \\ kh, & n_c = 3k; \\ (k+1)h, & n_c = 3k+1, \text{ or } n_c = 3k+2. \end{cases} \tag{4.2}$$

This operator representation is determined in the space $\ell^2(X)$ of square-summable sequences.

Proof. The commutation relations (3.11) implies that

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

Therefore the creation operator $\hat{B}$ has the form

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

Substituting the operator $\hat{B}$ into the Casimir operator $\hat{K} = 0$ (see (3.12)), we obtain $\beta(q, h)$. The restriction $\mathrm{Spec}(\hat{S}_j) = \{0, h, 2h, \dots\}$ gives the initial value q_0 of the discrete coordinate spectrum.

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

$$\frac{\varepsilon}{2}\beta(q + h, h)y(q + h) + \frac{\varepsilon}{2}\beta(q, h)y(q - h) + (aq^2 + bq)y(q) = \mathcal{E}y(q), \tag{4.3}$$

where $y(q) \in l^2(X)$, $\mathcal{E}$ is a spectral parameter.

We consider the spectral problem (4.3) in semiclassical approximation $h \ll 1$. General method of discrete WKB approximation is well developed (see, for instance, [11–13]), especially in applications to concrete quantum Hamiltonians [14–16]. The corresponding classical Hamiltonian mechanical systems are introduced by the Weyl symmetrized symbols (as in [13]). In our model the classical Hamiltonian $E(q, p)$, that is the symbol of $\hat{E}$, takes the form

$$E(q, p) = \varepsilon\beta(q + h/2, h)\cos(p) + aq^2 + bq. \tag{4.4}$$

The Hamiltonian $E(q, p)$ is a 2π-periodic function of the momentum p, and the classical phase space is a half-cylinder with $q > q_0 - h/2$.

The quantum energy levels which approximate the discrete spectrum of the Hamiltonian $\hat{E}$ up to $O(h^2)$ can be determined by the Planck–Bohr–Sommerfeld quantization rule [13, 14, 17]:

$$\frac{1}{2\pi}\oint_\gamma q\,dp = h(n + \sigma/2), \tag{4.5}$$

where n is an integer, γ is the periodic classical trajectory corresponding to an energy $\mathcal{E}$, the index $\sigma = 0$ if γ wraps around the phase space cylinder, or $\sigma = 1$ when γ contracts to a point.

The analysis of the phase portrait of the classical mechanical system with Hamiltonian $E(q, p)$ is based on the analysis of the turning points dependence on the energy $\mathcal{E}$. We define the turning point as a point on the classical trajectory, where the velocity $\dot{q} = E'_p$ is equal to zero. According to the form of the Hamiltonian (4.4), the turning points correspond to either points with momentum $p = 0$ or $p = \pi$. Therefore, coordinates of the turning points obey the equation

$$\pm\varepsilon\beta(q + h/2, h) + aq^2 + bq = \mathcal{E},$$

where the signs "+" and "−" correspond to turning points with $p = 0$ and $p = \pi$ respectively. Let $V_\pm(q) = \pm\varepsilon\beta(q + h/2, h) + aq^2 + bq$ be the potential curves, i.e. the curves of the turning points on (q, E) plane.

Let us analyze how classical trajectories depend on parameters of the Hamiltonian. Assume that the parameter d stays in a neighborhood of the value $d = 2$. Considering the asymptotic of $V_\pm(q)$ for large q we see that every classical trajectory is bounded if ε is sufficiently small (say $\varepsilon < 0.5$). Under this condition the potential curves $V_\pm(q)$ are close to two parabolas (see Fig. 2). We see that if $\varepsilon > 0$ (quadratic shape breaking) then there appears a separatrix and unstable equilibrium corresponding to the maximum of $V_-(q)$, the stable equilibrium corresponding to the maximum of

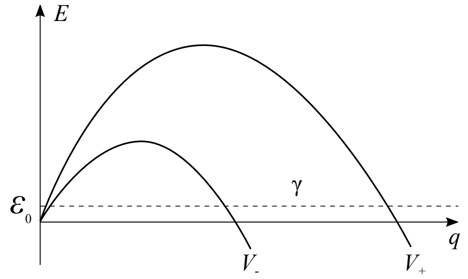

Fig. 2. Figure shows the turning points curves $V_{\pm}(q)$ in double-well regime. Here for simplicity we set $h = 0$, so the local energy minimum $q^* = q_0 = 0$. The classically allowed region lies between curves $V_{\pm}(q)$. There are two classically allowed regions corresponding to an energy $\mathcal{E}_0$, these regions are separated by the "barrier" $V_-(q)$.

$V_+(q)$ (the global maximum of the Hamiltonian E), and the local energy minimum $q = q^*$ with the energy $\mathcal{E}^* = V_-(q^*) = O(h)$. Thus for some small energies $\mathcal{E} > \mathcal{E}^*$, there appear two classical trajectories separated by classical barrier. We call it a "double-well' regime.

5. TUNNEL BILOCALIZATION AND INSTANTON

Suppose the parameters of the system are chosen so that the "double-well" regime is realized. Then the energy $\mathcal{E}^*$, that corresponds to the local energy minimum $q = q^*$, also corresponds to the periodic trajectory γ in region of lager values of coordinate q. We consider the quantum state of the lowest energy level $\mathcal{E}_0 > \mathcal{E}^*$ corresponding to the local minimum. This energy minimum is separated from the periodic trajectory by classical barrier.

The quantum tunnelling appears in discrete system (4.3) on very similar way as in the continuous Schrödinger equation (see, e.g., [15, 16, 18]), and it leads to the following effect. When we slightly change the parameter d of the system the quantum energy level $\mathcal{E}_0$ has many avoided crossings with energy levels of the bigger "well" and its state can be significantly localized near both the point q^* and the periodic trajectory γ.

Let φ_I and φ_{II} be the normalized approximate stationary states of $\hat{E}$ that are localized near the point $q = q^*$ and the periodic trajectory γ respectively. They can be rigorously defined as solutions of the difference equation (4.3) with an additional Dirichlet boundary condition on a point under the classical barrier.

Under variation of the parameter d in the avoided crossing effect two energy levels $\mathcal{E}_0$ and $\mathcal{E}_1$ of the operator $\hat{E}$ approach each other to a minimum distance Δ_{min} and then repel, while the corresponding precise stationary states $\psi_{0,1}$ form a linear combinations of the localized states φ_I and φ_{II}.

The following general relations holds [5, 19], if the stationary states has the form (2.2)

$$\psi_0 = g\varphi_I + \sqrt{1-g^2}\varphi_{II}, \qquad \psi_1 = \sqrt{1-g^2}\,\varphi_I - g\varphi_{II} \pmod{h^\infty} \tag{5.1}$$

where the parameter $g > 0$ is characterize how close we are to the avoided crossing point. Then the energy splitting is

$$|\mathcal{E}_1 - \mathcal{E}_0| = \frac{1 + O(\hbar)}{2g\sqrt{1-g^2}}\,\Delta_{min}, \tag{5.2}$$

The minimal splitting Δ_{min} corresponds to $g = 1/\sqrt{2}$, it is exponentially small as $h \to 0$:

$$\Delta_{min} = \exp\left(-\frac{S}{h}\,(1 + o(1))\right), \tag{5.3}$$

where S is called a tunnelling action.

It is known that the description of tunnelling dynamics of a quantum particle in the semiclassical approximation is closely related to the complexification of classical Hamiltonian equations (see the survey in [20–22]).

Let us consider the complexification of the Hamiltonian $E(q,p)$ and the corresponding trajectories of motion taking pure imaginary time $t=-i\tau$. We call the periodic complex trajectory $\tilde{\gamma}$ to be an *instanton* if it corresponds to the energy $\mathcal{E}_0$ and cross two real classical trajectories (see [16, 23]).

Theorem 5.1. *Suppose the parameter d vary in the fixed neighborhood of $d=2$, that corresponds to the double-well regime. Then, while we change the parameter d, there appears an avoided crossing of the lowest energy level $\mathcal{E}_0$ corresponding to energy minimum $q=q^*$ and the levels corresponding to trajectories γ. Under such a parameter tuning the two stationary states of $\hat{E}$ form a semiclassical bi-state and the corresponding 2-level system.*

The energy splitting have a form (5.2), (5.3), *where corresponding tunnelling action S is the action on the instanton:*

$$S=\frac{1}{2i}\int_{\tilde{\Sigma}} dp\wedge dq>0, \tag{5.4}$$

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

The derivation of the formula (5.4) is similar to that presented in [16]. Here we only mention that on the instanton trajectory $\tilde{\gamma}$ the momentum have a form $p=\pi+i\tilde{p}$ and coordinate q remains to be real and changing between two turning points.

To the trap configuration one may introduce an additional parameter by varying the strength of magnetic field. Then the coefficient b of the Hamiltonian (4.4) will depend on this parameter (see in Proposition 4). Thus in such a Penning trap via fine tuning of electric and magnetic fields we can obtain a continuous family of bi-state and 2-level systems.

APPENDIX

Let us denote by δ the real solution of the equation $(1+2\delta)\sqrt{1+\delta}=d$. Note that $\delta=\xi_1(d)^2$ in the symmetric case $T=1$ ($\varepsilon=0$). As $\varepsilon\ll 1$ the coefficients in (3.14) are given by the following formulas (all relations bellow are understood up to $O(\varepsilon^2)$):

$$\eta=\frac{3\big(20129-14428d^2-976d^4+4(12893-21363d^2+11805d^4)\delta-4(-7801+13604d^2)\delta^2\big)}{128d^2\big(-4-23d^2+27d^4-6(2+3d^2)\delta-8\delta^2\big)}\varepsilon,$$

$$\eta_{++}=\eta_{--}=-\frac{3\big(425-843d^2+468d^4-2(-542+1317d^2)\delta-4(-173+498d^2)\delta^2\big)}{16d^2(-6+6d^2+(-14+9d^2)\delta-8\delta^2\big)},$$

$$\eta_{00}=-\frac{1154-2289d^2+1260d^4-2(-1472+3567d^2)\delta-40(-47+135d^2)\delta^2}{24d^2\big(6(-1+d^2)+(-14+9d^2)\delta-8\delta^2\big)},$$

$$\begin{aligned}\eta_{+0}=\eta_{0+}=\eta_{-0}=\eta_{0-}&=-\frac{\sqrt{6}}{3}\eta_{+-}=-\frac{\sqrt{6}}{3}\eta_{-+}\\&=\frac{\sqrt{6}\big(667-1323d^2+756d^4-10(-170+417d^2)\delta-4(-271+786d^2)\delta^2\big)}{8d^2\big(6(-1+d^2)+(-14+9d^2)\delta-8\delta^2\big)},\end{aligned}$$

$$\eta_+ = \eta_- = \frac{15\big(-13+18d^2-26\delta-16\delta^2\big)}{16(5+6\delta)^2}$$
$$- \Big[\Big(\big(5277-1334\sqrt{6}+9(-1163+294\sqrt{6})d^2-108(-55+14\sqrt{6})d^4$$
$$+2\big(2(3363-850\sqrt{6})+3(-5487+1390\sqrt{6})d^2\big)\delta$$
$$+4\big(2145-542\sqrt{6}+6(-1035+262\sqrt{6})d^2\big)\delta^2\big)h\Big)\Big]\Big/$$
$$\Big(32d^2\big(6(-1+d^2)+(-14+9d^2)\delta-8\delta^2\big)\Big),$$

$$\eta_0 = -\frac{5\sqrt{6}\big(-13+18d^2-26\delta-16\delta^2\big)}{16(5+6\delta)^2}$$
$$+\Big[\Big(2(-577+2001\sqrt{6})-21(-109+378\sqrt{6})d^2+252(-5+18\sqrt{6})d^4$$
$$+2\big(4(-368+1275\sqrt{6})-3(-1189+4170\sqrt{6})d^2\big)\delta$$
$$-8\big(235-813\sqrt{6}+9(-75+262\sqrt{6})d^2\big)\delta^2\Big)h\Big]\Big/$$
$$\Big(48d^2\big(6(-1+d^2)+(-14+9d^2)\delta-8\delta^2\big)\Big),$$

$$\zeta = \frac{5(6-\sqrt{6})(-13+18d^2-26\delta-16\delta^2)h}{32(5+6\delta)^2}$$
$$+\Big[\Big(-2(19498-6003\sqrt{6})+3(25783-7938\sqrt{6})d^2-36(1223-378\sqrt{6})d^4$$
$$+10\big(20(-497+153\sqrt{6})+3(8117-2502\sqrt{6})d^2\big)\delta$$
$$-8\big(7924-2439\sqrt{6}-9(2551-786\sqrt{6})d^2\big)\delta^2\Big)h^2\Big]\Big/$$
$$\Big(288d^2\big(6(-1+d^2)+(-14+9d^2)\delta-8\delta^2\big)\Big).$$

The coefficients in formula (3.15) are determined $modO(\varepsilon^2)$ by

$$\mu = \frac{\eta}{\epsilon}, \qquad a = \frac{1}{\mu}\Big(5\eta_{++}+3\eta_{+-}\Big),$$

$$b = \frac{1}{\mu}\Big(3h(n_- - 3n_+)\eta_{++} + 4\eta_+ + h\big(n_- - 3n_+ - \frac{4}{3}\sqrt{6}\,n_0\big)\eta_{+-}\Big),$$

$$c = \frac{1}{6\mu}\Big(3h^2(n_- - 3n_+)^2\eta_{++} - 2h(n_- - 3n_+)(\sqrt{6}\,h\,n_0\eta_{+-} - 3\eta_+) + 3h\,n_0(2+hn_0)\eta_0 + 6\zeta\Big).$$

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