Monodromy, diabolic points, and angular momentum coupling

D. A. Sadovskií and B. I. Žhilinskií [1]

Université du Littoral, BP 5526, 59379 Dunkerque Cedex, France

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Abstract

Monodromy, or the most basic obstruction to global action-angle coordinates is shown to be present in the well known problem of two coupled angular momenta. It is also shown that in the corresponding quantum problem monodromy manifests itself as the redistribution of energy levels between different multiplets of the quantum spectrum.

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1 Introduction

Advances in classical dynamical theory and their relevance to quantum mechanics can be often best understood on simple examples. In the present note we provide an example that highlights certain global aspects of classical integrable systems [1], especially the obstruction to the existence of global action-angle variables known as monodromy [2].

[1] e-mail: zhilin@univ-littoral.fr

1.1 Hamiltonian, notation, symmetry

We consider a simple problem of two coupled angular momenta (two rotors) $\mathbf{S}$ and $\mathbf{N}$ [3] with the Hamiltonian function

$$H = \frac{1-\gamma}{|\mathbf{S}|} S_z + \frac{\gamma}{|\mathbf{N}||\mathbf{S}|} (\mathbf{N} \cdot \mathbf{S}), \quad 0 \leq \gamma \leq 1, \tag{1}$$

and coupling parameter γ. We study this problem as a one-parameter family for arbitrary *fixed* amplitudes $|\mathbf{N}|$ and $|\mathbf{S}|$ of the angular momenta and focus on the case $|\mathbf{N}| > |\mathbf{S}|$. Our parameterization of (1) is such that the region of classically admissible energies remains the same for all γ in the interval $[0, 1]$. We note that the Hamiltonian (1) (or slight modifications of it) serves as an effective quantum operator in many fundamental physical applications. We return briefly to this in sec. 6.

A concise simultaneous presentation of quantum and classical problems with Hamiltonian (1), each with its own traditional notation, requires certain compromise and intuition based on the context. So in this note we do not use different notation for quantum and classical operators, neither do we distinguish functions and their values. We will denote the quantum numbers of angular momenta as N and S. These numbers take integer or half-integer values, while classical amplitudes $|\mathbf{N}|$ and $|\mathbf{S}|$ of the momenta equal $\sqrt{N(N+1)}$ and $\sqrt{S(S+1)}$, respectively. Such definition improves the quantum classical correspondence at low quantum numbers; it becomes unimportant in the classical limit of large S and N.

The symmetry of our problem is largely responsible for the qualitative phenomena we observe and thus is of primary importance in the analysis. The Hamiltonian (1) is invariant with respect to rotations around axis z (simultaneous rotations around axes N_z and S_z in the $\mathbf{N}$ and $\mathbf{S}$ spaces) which form the group $SO(2)$. The corresponding integral of motion, $J_z = N_z + S_z$, is the projection of the total angular momentum $\mathbf{J}$ on axis z. There is also an additional finite symmetry group $Z_2 = \{I, T_v\}$ whose nontrivial operation $T_v = T \circ \sigma_v$ is a product of the momentum reversal $T : (\mathbf{N}, \mathbf{S}) \to (-\mathbf{N}, -\mathbf{S})$ (which can be regarded as "time reversal") and the spatial reflection in any of the vertical planes that contain axis z. An example of the Z_2 action is $(N_x, N_y, N_z) \to (N_x, -N_y, N_z)$, a combination of T and the reflection in the xz plane. The complete symmetry group $G = SO(2) \wedge Z_2$ is an extension of $SO(2)$ and is exactly the same as the symmetry group of the hydrogen atom in parallel electric and magnetic fields [4].

1.2 *Outline of the analysis*

Our main idea is to compare global features of the one-parameter family of completely quantum problems with Hamiltonian (1) (where both angular momenta are quantum operators), to the features of the corresponding family in the "semi-quantum" approach (where one angular momentum, such as "spin" $\mathbf{S}$, is a quantum operator while $\mathbf{N}$ is a 3-vector of classical dynamical variables), and also to the features of the family of completely classical problems (where both $\mathbf{N}$ and $\mathbf{S}$ represent classical variables). We follow the general scheme of comparative qualitative quantum-classical analysis [4–6] where structures in the quantum spectrum, such as multiplets of quasi-degenerate levels[11], are associated with topology and symmetry properties of the corresponding classical dynamical system.

Our quantum study (sec. 2) focuses on the well known qualitative phenomenon of the energy level redistribution between the multiplets. In our example, the number of levels in the multiplets changes when the value of γ varies from 0 to 1 and a transition from a spectrum of a problem with uncoupled momenta to that characteristic for a problem with coupled momenta occurs. As in the earlier paper [3], we relate this redistribution phenomenon to conical intersections of classical energy surfaces which replace the multiplets in the semi-quantum approach (sec. 3). For our choice of γ this intersection, or "diabolic point" occurs when $\gamma = 1/2$ and the redistribution takes place when the values of γ are close to $1/2$.

The main contribution of this paper may be found in sec. 4 where we show that for all values of parameter γ in an open sub-interval $\mathcal{I}$ of $[0, 1]$ containing $1/2$ the classical problem has monodromy. Furthermore, we find that in the limit $|\mathbf{S}|/|\mathbf{N}| \to 0$ the monodromy interval $\mathcal{I}$ shrinks to the point $\gamma = 1/2$. Thus the three phenomena are intrinsically related. In sec. 5 we demonstrate that quantum implications of monodromy in our example are identical to those found in other systems [7–9].

2 Quantum description

Quantum problems similar to (1) can be found in many textbooks [10]. For arbitrary quantum numbers S and N the space of $(2N + 1)(2S + 1)$ wavefunctions factors into a sum of subspaces of functions with given quantum number J_z. (For $S \leq N$ the maximal dimension of each summand is $2S + 1$.) The eigenvalues of the Hamiltonian (1) are obtained by matrix diagonalization. The quantum number J_z does not characterize the multiplet structure of the quantum spectrum of (1) because multiplets consist of states with different J_z.

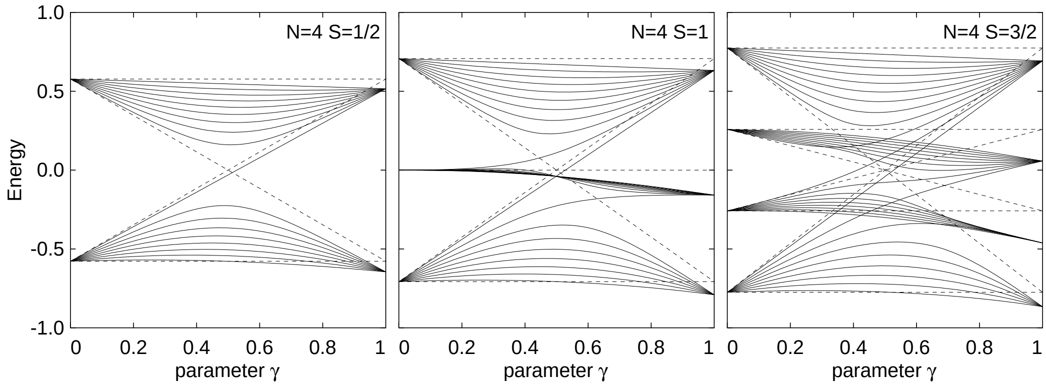

Fig. 1. Quantum energy spectrum (solid lines) for two-level ($S = 1/2$), three-level ($S = 1$), and four-level ($S = 3/2$) problems with Hamiltonian (1) and $N = 4$. Extrema of corresponding semi-quantum energies (2) are shown by dashed lines.

This structure can be easily understood near the two limits $\gamma = 0$ and $\gamma = 1$ using appropriate good (approximate) quantum numbers.

When γ is close to 0 we use the eigenvalues of S_z and N_z as good quantum numbers. S_z characterizes the multiplet structure. There are $2S+1$ multiplets or quasi-degenerate groups of levels with $2N+1$ levels in each group [11]. Within each such multiplet the levels have the same value of S_z and are distinguished by the value of N_z. The energy of each multiplet depends linearly on S_z. The first order splitting of levels within multiplets depends linearly on N_z. We say that N_z describes the internal structure of multiplets. When γ is close to 1 we use a different pair of good quantum numbers (J, J_z). Here $\mathbf{J} = \mathbf{N} + \mathbf{S}$ is the total angular momentum and J_z is the projection of $\mathbf{J}$ on the z-axis. In this limit J describes the multiplet structure. For $N \geq S$, there are $2S + 1$ quasi-degenerate multiplets labeled by $J = N + S, N + S - 1, \ldots, N - S$ with energy approximately increasing as $\mathbf{J}^2 = J(J + 1)$. Within each multiplet, levels with the same J are distinguished by J_z so that the first order splitting is a linear function of J_z [10].

Transformation of the eigenfunctions of the Hamiltonian (1) from the limit $\gamma = 0$ to the limit $\gamma = 1$ is a well known transformation from the uncoupled to coupled basis for two angular momenta, $|NN_zSS_z\rangle \to |NSJJ_z\rangle$. When $N \geq S$, the number of multiplets in the two limits is the same but the number of levels within each multiplet is different. Consequently, a number of levels is redistributed among the multiplets [11] at intermediate values of the control parameter γ. The redistribution phenomenon is illustrated in Figure 1 on the example of $S = 1/2$, 1, 3/2 and $N = 4$. It is most clearly seen for the case $S = 1/2$ analyzed earlier in [3,11].

3 Semi-quantum description and diabolic points

The "semi-quantum" approach is based on the idea that different multiplets or branches [11] with sufficiently many quantum levels can be considered as individual (interacting) quantum states whose internal structure can be analyzed using a classical Hamiltonian. In particular, such approach has been applied to the description of rotation-vibration energy levels, see references cited in [5,6].

In our case, if $S \ll N$ the "spin" $\mathbf{S}$ remains a quantum operator, while $\mathbf{N}$ becomes a classical vector of angular momentum. Calculation of energies is straightforward as soon as we realize that the semi-quantum Hamiltonian (1) is a linear combination of quantum operators S_x, S_y, S_z whose coefficients are functions of classical variables (N_x, N_y, N_z) and parameters γ, $|\mathbf{N}|$, and $|\mathbf{S}|$. We rotate (S_x, S_y, S_z) so that in the new frame $(S_{x'}, S_{y'}, S_{z'})$ our Hamiltonian depends only on $S_{z'}$, the projection of $\mathbf{S}$ on the new axis z'. The energy

$$E_{S_{z'}} = \frac{S_{z'}}{|\mathbf{S}|} \left| \sqrt{1 + 2\gamma(\gamma - 1)\left(1 - \frac{N_z}{|\mathbf{N}|}\right)} \right| \tag{2}$$

of the $2S+1$ multiplets (branches) is labeled by $S_{z'} = -S, -S{+}1, \ldots, S{-}1, S$ (cf. eq. (5) of [3]). Each of these multiplets is now regarded as a classical dynamical system with Hamiltonian (2) and dynamical variables (N_x, N_y, N_z) in an Euclidean ambient space R_3. The phase space is a 2-sphere defined in this R_3 as a level set of $|\mathbf{N}|$.

The Hamiltonians (2) can themselves be represented as deformed spheres in the same space R_3 and are often called *energy surfaces*. These surfaces have a maximum at $N_z = |\mathbf{N}|$ and a minimum at $N_z = -|\mathbf{N}|$ for all values of γ in the interval $(0, 1)$ except $\gamma = 1/2$ where they have a singularity at $N_z = -|\mathbf{N}|$. At this "diabolic" point *all* energy surfaces have the same energy and form one many-sheeted surface. They do not represent $2S+1$ individual multiplets but rather reflect the fact that a certain number of levels is redistributed among the multiplets. Such dynamical interpretation of the energy level redistribution was proposed in [3,11] based on the example of $S = 1/2$ (fig. 1, left). The universal character of this phenomenon and the relation between the type of singularity and the number of levels transferred was subsequently studied in [12,13].

The strikingly clear correspondence of the redistribution and the diabolic point in the two state (two surface) case with $S = 1/2$ suggests that a full classical analysis of these phenomena should be conducted in the limit where N and S are both large *and* $|\mathbf{S}|/|\mathbf{N}| \to 0$. Note, that in this classical limit, the disagreement between the semi-quantum energy surfaces and quantum multiplets for

$\gamma \approx 1$ (fig. 1) vanishes as the number of redistributed levels (the difference in the number of levels) relative to the total number of levels in the multiplet becomes negligible. (For instance, the central multiplet with $J \sim N$ has the largest discrepancy which is $-\frac{1}{2}|\mathbf{S}|/|\mathbf{N}|$ when $\gamma = 1$ and converges to 0.)

4 Classical model and monodromy

Since $|\mathbf{S}|$ and $|\mathbf{N}|$ are conserved, the phase space of the classical problem is $S_2 \times S_2$, the product of two spheres, and the number of degrees of freedom equals 2. Each sphere S_2 is defined in the respective 3-space (S_x, S_y, S_z) and (N_x, N_y, N_z) as

$$S_x^2 + S_y^2 + S_z^2 = |\mathbf{S}|^2, \quad N_x^2 + N_y^2 + N_z^2 = |\mathbf{N}|^2. \tag{3}$$

Both $\mathbf{N}$ and $\mathbf{S}$ generate each a standard $so(3)$ algebra, so that

$$\{N_a, N_b\} = \varepsilon_{abc} N_c, \quad \{S_a, S_b\} = \varepsilon_{abc} S_c, \quad \{N_a, S_b\} = 0 \ \ \forall\, a, b.$$

Furthermore, as already mentioned in sec. 1.1, the diagonal $SO(2)$ symmetry of our Hamiltonian (1) results in the second integral of motion

$$J_z = S_z + N_z, \quad \{H, J_z\} = 0. \tag{4}$$

The problem is, therefore, Liouville integrable.

The diagonal action of $SO(2)$ on $S_2 \times S_2$ has four fixed points with $S_x = S_y = N_x = N_y = 0$. As a consequence, we can only remove this symmetry by means of *singular reduction* [1]. This results in a family of reduced phase spaces P_{J_z} parameterized by the value of J_z, such that $|J_z| \leq |\mathbf{N}| + |\mathbf{S}|$. Several members in this family P_{J_z} are singular spaces. They are of primary interest to our study. To find these spaces we use the formal geometric approach based on the orbit space construction [4,14] and the standard theory of invariants [15–17].

4.1 Reduction of symmetries, orbit space $\mathcal{O}$

We reduce the diagonal action of $SO(2)$ on the four dimensional phase space $S_2 \times S_2$ by mapping each orbit of the $SO(2)$ action onto a space of orbits $\mathcal{O}$ of dimension 3. These orbits correspond to different relative configurations of vectors $\mathbf{S}$, $\mathbf{N}$, and the unit vector $\mathbf{n}_z$ which defines the direction of axis

z (the axis of symmetry). The orbits can be labeled by the values of three algebraically independent invariants

$$S_z, \quad N_z, \quad \xi = \mathbf{N} \cdot \mathbf{S}, \tag{5}$$

that is, by the projection of vectors $\mathbf{S}$ and $\mathbf{N}$ on axis z, and the angle between them. Alternatively, we can use

$$K_z = S_z - N_z, \quad J_z, \quad \xi. \tag{6}$$

To label the orbits of the $SO(2)$ action uniquely we need an additional linearly independent invariant

$$\sigma = \mathbf{n}_z \cdot (\mathbf{S} \wedge \mathbf{N}), \tag{7}$$

which is the z-projection of the vector product of $\mathbf{S}$ and $\mathbf{N}$. This invariant depends algebraically on (S_z, N_z, ξ), namely

$$\sigma^2 + (\xi - N_z S_z)^2 - (\mathbf{S}^2 - S_z^2)(\mathbf{N}^2 - N_z^2) = 0, \tag{8}$$

To distinguish the orbits we need only specify its sign [18].

The action of the additional Z_2 symmetry explained in sec. 1.1 can now be reduced straightforwardly. We remark that ξ, S_z, and N_z (or J_z and K_z) are invariants of the Z_2 action, while σ is a covariant, $T_v : \sigma \to -\sigma$. Therefore, the orbits of the $SO(2) \wedge Z_2$ action are labeled uniquely by (S_z, N_z, ξ). For each such orbit we can find the value of $|\sigma|$. If $|\sigma| = 0$ we are dealing with a single $SO(2)$ orbit, either a fixed point (with stabilizer $SO(2) \wedge Z_2$), or a circle $S_1 \subset S_2 \times S_2$ (with stabilizer Z_2). Otherwise the $SO(2) \wedge Z_2$ orbit is a pair of $SO(2)$ orbits, that is, a pair of circles (generic orbits with trivial stabilizer).

It follows that the set $\mathcal{O}$ of all orbits of the $SO(2) \wedge Z_2$ action can be defined as an algebraic variety in the 3-space (S_z, N_z, ξ). In fact we can show that $\mathcal{O}$ is a closed ball in R_3 whose boundary is a topological 2-sphere with four singular points at the fixed points of the $SO(2)$ action. For points in the boundary we have $\sigma = 0$. Equation (8) with $\sigma = 0$ defines a surface in R_3. In the normalized variables

$$-1 \leq S_z/|\mathbf{S}| \leq 1, \quad -1 \leq N_z/|\mathbf{N}| \leq 1, \quad -1 \leq \xi/(|\mathbf{N}||\mathbf{S}|) \leq 1,$$

this surface remains the same for any $|\mathbf{N}|$ and $|\mathbf{S}|$, see fig. 2, left. Specifically, this surface is a tetrahedron whose edges are rounded except at the vertices A, B, C, and D which are singular points corresponding to the fixed points

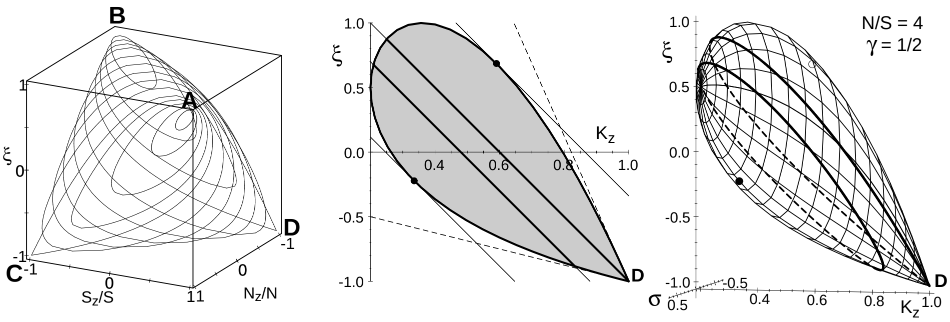

Fig. 2. Space $\mathcal{O}$ of all orbits of the $SO(2)\wedge Z_2$ action on $S_2\times S_2$ (left) sliced by planes $J_z = -4.5, -4, \ldots, 4, 4.5, 4.8$. Singular space of orbits $\mathcal{O}_{J_z}$ at fixed $J_z = |\mathbf{S}| - |\mathbf{N}|$ (center) and the corresponding phase space P_{J_z} (right) intersected by constant level sets of Hamiltonian (1) with $\gamma = 1/2$. In all cases $|\mathbf{N}| = 4$, $|\mathbf{S}| = 1$, and axes correspond to normalized coordinates $\xi/(|\mathbf{N}||\mathbf{S}|)$, $\sigma/(|\mathbf{N}||\mathbf{S}|)$, and $K_z/(|\mathbf{N}| + |\mathbf{S}|)$.

Table 1
Critical orbits of the $SO(2) \wedge Z_2$ action on the phase space $S_2 \times S_2$.

Orbit	N_z	S_z	ξ	Energy	J_z	K_z
A	$\lvert\mathbf{N}\rvert$	$\lvert\mathbf{S}\rvert$	$\lvert\mathbf{S}\rvert\lvert\mathbf{N}\rvert$	1	$\lvert\mathbf{N}\rvert + \lvert\mathbf{S}\rvert$	$-\lvert\mathbf{N}\rvert + \lvert\mathbf{S}\rvert$
B	$-\lvert\mathbf{N}\rvert$	$-\lvert\mathbf{S}\rvert$	$\lvert\mathbf{S}\rvert\lvert\mathbf{N}\rvert$	$2\gamma - 1$	$-\lvert\mathbf{N}\rvert - \lvert\mathbf{S}\rvert$	$\lvert\mathbf{N}\rvert - \lvert\mathbf{S}\rvert$
C	$\lvert\mathbf{N}\rvert$	$-\lvert\mathbf{S}\rvert$	$-\lvert\mathbf{S}\rvert\lvert\mathbf{N}\rvert$	-1	$\lvert\mathbf{N}\rvert - \lvert\mathbf{S}\rvert$	$-\lvert\mathbf{N}\rvert - \lvert\mathbf{S}\rvert$
D	$-\lvert\mathbf{N}\rvert$	$\lvert\mathbf{S}\rvert$	$-\lvert\mathbf{S}\rvert\lvert\mathbf{N}\rvert$	$1 - 2\gamma$	$-\lvert\mathbf{N}\rvert + \lvert\mathbf{S}\rvert$	$\lvert\mathbf{N}\rvert + \lvert\mathbf{S}\rvert$

(critical orbits) of the diagonal $SO(2)$ action, that is, to the *equilibria* of (1). The position and the corresponding value of the Hamiltonian (1) at the vertices is given in table 1. The lines connecting the vertices remain on the surface. The space of $SO(2) \wedge Z_2$ orbits $\mathcal{O}$ is all points on and inside the bounding surface.

4.2 Fully reduced space $\mathcal{O}_{J_z}$ and reduced phase space P_{J_z}

Dynamically we are interested in the sets of orbits of the $SO(2) \wedge Z_2$ action with the same value of the integral of motion J_z. These are a family of planar slices $\mathcal{O}_{J_z}$ of the orbit space $\mathcal{O}$ illustrated in fig. 2, left. We call them *fully reduced spaces*. For maximum and minimum values of $J_z = \pm(|\mathbf{N}| + |\mathbf{S}|)$ the space $\mathcal{O}_{J_z}$ is a point (A and B in fig. 2), for $J_z = \pm(|\mathbf{N}| - |\mathbf{S}|)$ it is a disk with one singular point on the boundary (either C or D). In the special case $|\mathbf{N}| = |\mathbf{S}|$, the space $\mathcal{O}_{J_z}$ at $J_z = 0$ has two singular points, and to avoid this case we will assume $|\mathbf{N}| > |\mathbf{S}|$ for the rest of the paper. For all other *regular* values of J_z the space $\mathcal{O}_{J_z}$ is a smooth 2-disk.

For our choice of $|\mathbf{N}| > |\mathbf{S}|$ and $0 < \gamma < 1$ the singular space $\mathcal{O}_{J_z}$ with $J_z = |\mathbf{S}| - |\mathbf{N}|$ becomes crucial to the analysis. An example of such singular space is shown in fig. 2, center. The most important characteristics of this space is the slope of the two lines tangent to its boundary ($\sigma = 0$) at the singular point D (dashed lines in fig. 2). The slope of these lines is given by

$$\tan\alpha_{1,2} = -\frac{1}{2}\left(\sqrt{|\mathbf{N}|} \pm \sqrt{|\mathbf{S}|}\right)^2. \tag{9}$$

(In the normalized coordinates of fig. 2, center, the slope is $\frac{|\mathbf{N}|+|\mathbf{S}|}{|\mathbf{N}||\mathbf{S}|}\tan\alpha$). It can be seen that in the limit $|\mathbf{S}|/|\mathbf{N}| \to 0$ our special singular space degenerates to a line with $\tan\alpha = -\frac{1}{2}|\mathbf{N}|$. The same conclusion can be obtained using intersections of the full orbit space $\mathcal{O}$ (fig. 2, left) and planes representing constant level sets of H and J_z. In the limit $|\mathbf{S}|/|\mathbf{N}| \to 0$ these planes are parallel to the plane $(\xi, S_z = (K_z + J_z)/2)$ and the singular space with $N_z = J_z = -|\mathbf{N}|$ is the straight line BD, which is formed when the plane $N_z/|\mathbf{N}| = -1$ is tangent to the bounding surface $\sigma^2 = 0$. (Indeed, the slope of the two tangent lines in this representation is $\frac{|\mathbf{S}|}{|\mathbf{N}||\mathbf{S}|}\frac{d\xi}{dK_z}\frac{dK_z}{dS_z} = \frac{2}{|\mathbf{N}|}\tan\alpha \to -1$).

The *reduced phase space* P_{J_z} is the set of all orbits of the diagonal $SO(2)$ action having the same value of J_z. Therefore, the fully reduced space $\mathcal{O}_{J_z}$ is the orbit space P_{J_z}/Z_2. A point in the boundary of $\mathcal{O}_{J_z}$ ($\sigma = 0$) lifts to a point in P_{J_z}, while a point in the interior ($\sigma \neq 0$) corresponds to two points on P_{J_z}. This suggests that topologically P_{J_z} is a 2-sphere. Indeed, we can see that the two factors in the last term in the left hand side of eq. (8) are always positive. This equation defines P_{J_z} as a smooth 2-sphere in the space of dynamical variables (ξ, σ, K_z) for all regular values of J_z. Otherwise P_{J_z} is a sphere with one singular point shown in fig. 2, right, or a point. To complete our singular reduction we note that (K_z, σ, ξ) generate a Poisson algebra which restricts naturally to a Poisson algebra on P_{J_z}, where the expression in the left hand side of eq. (8) is a Casimir function.

4.3 Level sets of H, energy-momentum map $\mathcal{E}M$

The fully reduced space $\mathcal{O}_{J_z}$ is the most natural tool for the qualitative analysis of the Hamiltonian (1), which is itself a function of dynamical variables ξ, K_z and J_z—all invariants of the $SO(2) \wedge Z_2$ action—and parameters γ, $|\mathbf{N}|$ and $|\mathbf{S}|$. Of course, for the reduced Hamiltonian

$$\mathcal{H}_{J_z}(\xi, K_z) = \frac{(1-\gamma)}{2|\mathbf{S}|}(K_z + J_z) + \frac{\gamma}{|\mathbf{N}||\mathbf{S}|}\xi, \tag{10}$$

the fixed value of J_z is also a *parameter*. The level sets of (10) are straight lines whose intersection with $\mathcal{O}_{J_z}$ is the image of dynamically invariant subsets

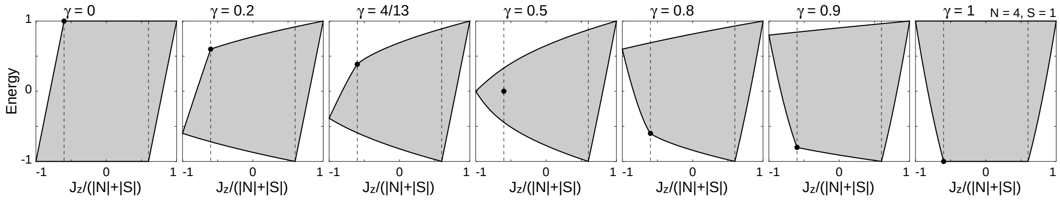

Fig. 3. Range of the energy momentum map $\mathcal{E}M$ for Hamiltonian (1) with different values of parameter γ and $|\mathbf{N}|/|\mathbf{S}| = 4$.

M_{J_z} of $S_2 \times S_2$ with fixed J_z and H. Certain level sets of H can intersect $\mathcal{O}_{J_z}$ at a single point which is one of the critical orbits A, B, C, or D. Such sets correspond to equilibrium points. Three other qualitatively different possibilities are illustrated in fig. 2, center. They are (i) a point with $\sigma = 0$ where the level set is tangent to the boundary of $\mathcal{O}_{J_z}$; (ii) a regular interval closed by two points with $\sigma = 0$; and (iii) an interval whose boundary contains a critical point (point D if $|\mathbf{N}| > |\mathbf{S}|$ and $0 \leq \gamma \leq 1$). The level sets of the first kind correspond to the maximum and minimum energy H at given J_z, i.e., to the *relative equilibria* of (1). The regular level sets of $\mathcal{H}_{J_z}$ correspond to intermediate energies. The level set of the third kind exists only when

$$\frac{|\mathbf{N}|}{2|\mathbf{N}| + |\mathbf{S}| + 2\sqrt{|\mathbf{N}||\mathbf{S}|}} \leq \gamma \leq \frac{|\mathbf{N}|}{2|\mathbf{N}| + |\mathbf{S}| - 2\sqrt{|\mathbf{N}||\mathbf{S}|}}, \tag{11}$$

that is, when the slope of the constant level sets of $\mathcal{H}_{J_z}$ lies within the interval defined by eq. (9). In the limit $|\mathbf{S}|/|\mathbf{N}| \to 0$, this interval shrinks towards one point $\gamma = 1/2$.

To understand how different invariant subspaces M_{J_z} "fit together" we consider the following energy-momentum map

$$\mathcal{E}M_\gamma \ : \ S_2 \times S_2 \to R_2 \ : \ p \to (H_\gamma(p), J_z(p)). \tag{12}$$

Each value of $\mathcal{E}M$, a point in the plane R_2, corresponds to the set of all points p in the initial phase space $S_2 \times S_2$ where energy $H(p)$ and momentum $J_z(p)$ have given values (h, j). In other words, the dynamically invariant set

$$M_{J_z} \subseteq S_2 \times S_2 = \mathcal{E}M_\gamma^{-1}(h, j)$$

is a fiber of $\mathcal{E}M$. Level sets of $\mathcal{H}_{J_z}$ on $\mathcal{O}_{J_z}$ map to points in the range of $\mathcal{E}M$ shown for different parameters γ as a shaded area in fig. 3. Values $\mathcal{E}M(A)$, $\mathcal{E}M(B)$, $\mathcal{E}M(C)$, $\mathcal{E}M(D)$, and points in the boundary of the range of $\mathcal{E}M$ are critical values of $\mathcal{E}M$ (cf. Chap. I.2 and IV.3 of [1]). All other points are regular values. In the limit $\gamma = 0$ and $\gamma = 1$ the range of $\mathcal{E}M$ is a parallelogram and a trapezoid with slightly curved lateral sides, respectively, whose vertices correspond to the four equilibria listed in table 1. As the value of γ changes from 0 to 1, the points $\mathcal{E}M(D)$ and $\mathcal{E}M(C)$ move. When γ lies in the interval (11), the point $\mathcal{E}M(D)$ becomes an *isolated critical value* of $\mathcal{E}M_\gamma$. This suggests that in this interval of parameter values the problem has monodromy.

4.4 Reconstruction of the level sets of H, monodromy

To understand monodromy we find the topology of all fibers of $\mathcal{E}M$, that is, we reconstruct the invariant manifolds M_{J_z}. To this end we follow a combination of the energy-momentum and reduction maps. From a point (h, j) in the range of $\mathcal{E}M_\gamma$ we go to the level set of $\mathcal{H}_{J_z} = h$ on $\mathcal{O}_{J_z}$ with $J_z = j$ and on P_{J_z}. We then lift this level set to the initial space $S_2 \times S_2$. By the Arnol'd-Liouville theorem (see [1], notes on p. 408), each regular value (h, j) of $\mathcal{E}M$ lifts to a 2-torus T_2 in the initial phase space $S_2 \times S_2$. Indeed, a regular value of $\mathcal{E}M$ lifts to a regular closed interval on $\mathcal{O}_{J_z}$, which in turn becomes a regular circle S_1 on P_{J_z} (see fig. 2, right). This circle is contractible to a regular point in P_{J_z}, and thus is the base of a trivial bundle $T_2 = S_1 \times S_1$ in $S_2 \times S_2$. We also find that the critical values $\mathcal{E}M(A)$, $\mathcal{E}M(B)$, $\mathcal{E}M(C)$ correspond to equilibrium points on $S_2 \times S_2$. The same happens to $\mathcal{E}M(D)$ when γ lies outside the interval (11). Other points in the boundary of the range of $\mathcal{E}M$ (maximum and minimum energy at given J_z) lift to points on $\mathcal{O}_{J_z}$ and P_{J_z} (Z_2 symmetric relative equilibria with $\sigma = 0$) and then to periodic orbits on $S_2 \times S_2$.

When $\mathcal{E}M(D)$ is an isolated critical value (as in fig. 3, center) the fiber of $\mathcal{E}M_\gamma$ over $\mathcal{E}M(D)$ is a *pinched torus*, that is, a homoclinic connection of stable and unstable manifolds of D. To see this we reconstruct the corresponding level set on the singular space $P_{|\mathbf{S}|-|\mathbf{N}|}$ (fig. 2, right). This set is a topological circle consisting of an open interval $\mathcal{C}$ of regular points and a singular point p. The interval $\mathcal{C}$ lifts to a cylinder $\mathcal{C} \times S_1 \subset S_2 \times S_2$, while p goes to point D. Thus each end of the cylinder is pinched to a point and the two points are identified. It is a theorem that existence of such isolated pinched torus implies that the energy-momentum map has monodromy [19].

5 Quantum monodromy

In the presence of monodromy [2,1], the 2-torus bundle over a circle S_1 in the open domain of regular values of the energy-momentum map $\mathcal{E}M$, which loops around the isolated critical value $\mathcal{E}M(D)$ (fig. 4), is non-trivial, that is, $\mathcal{E}M^{-1}(S_1)$ is not $S_1 \times T_2$. As a consequence, there is no unique way to label all invariant tori surrounding the pinched torus, that is, no action-angle variables can be introduced in the neighborhood of D. This fact is used in [7–9] to

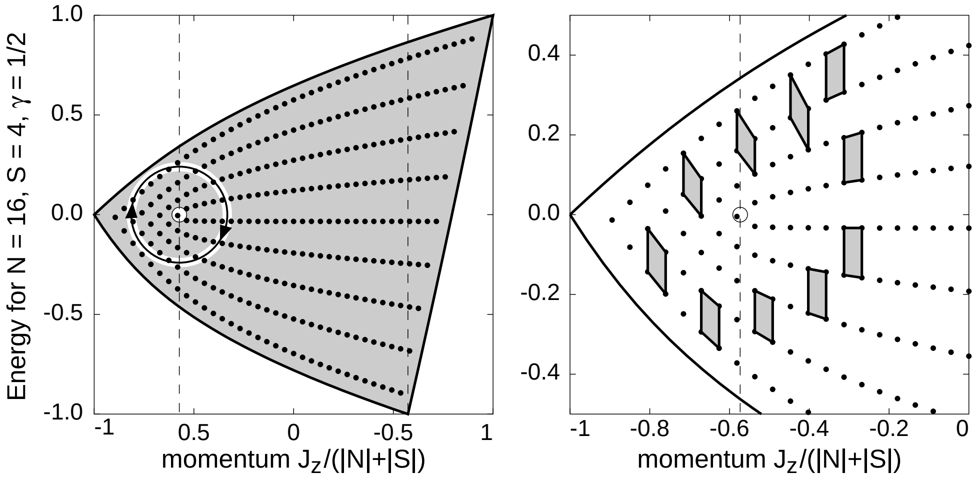

Fig. 4. Quantum energy levels for $N = 16, S = 4$ and $\gamma = 1/2$ plotted in the range of the corresponding classical energy-momentum map $\mathcal{E}M$. The value $\mathcal{E}M(D)$ corresponding to the pinched torus lies in the center of the white disk.

manifest quantum monodromy.

Following the same approach for the Hamiltonian (1), we superimpose the range of $\mathcal{E}M$ and the 2D-lattice of points representing the energy and momentum of quantum levels, that is, the values of $\mathcal{E}M$ on the EBK tori. We then vary the value of parameter γ and consider qualitative changes of the lattice. It is clear that in the two limits the lattices are regular, their points lie on $2S + 1$ horizontal lines of constant energy, so that there are $2N + 1$ points per line when $\gamma = 0$ and a varying number when $\gamma = 1$ (imagine lattices on the leftmost and rightmost plots in fig. 3). As long as γ stays outside the monodromy interval $\mathcal{I}$ in (11), lattices can be obtained by a smooth deformation of the corresponding limit lattices (consider lattices for the second left and right plots in fig. 3). The qualitative change occurs when γ enters $\mathcal{I}$ in (11). In this case the lattice has a point defect located at the value of $\mathcal{E}M$ on the pinched torus. Figure 4 shows such lattice for quantum numbers $N = 16$, $S = 4$ (such that the ratio $|\mathbf{N}|/|\mathbf{S}|$ is close to the one in fig. 3) and parameter $\gamma = 1/2$.

As we can see in fig. 4, quantum energy levels within an open disk $\mathcal{R}$ in the regular domain of $\mathcal{E}M$ can be ordered using a set of integer quantum numbers (i, j), the values of the two action integrals on the corresponding EBK tori. In other words, quantum states with the values of energy H and momentum J_z within $\mathcal{R}$ (i.e., locally) form a regular lattice on $\mathcal{R}$. Four quantum states (i, j), $(i, j + 1)$, $(i + 1, j)$, $(i + 1, j + 1)$, define vertices of an elementary cell of this lattice. Moving such cell around within $\mathcal{R}$ we always come back to the *same* cell. If, however, we quit $\mathcal{R}$ and move our cell along a path around the isolated critical value $\mathcal{E}M(D)$ as shown in fig. 4, right, by a series of shaded cells which correspond to the closed path in fig. 4, left, we come back with a different elementary cell which is related to the initial cell by a unimodular transformation over integers. (In fig. 4, right, we start with a "parallelogram" and come back with a "rhombus".) It follows that in the case with monodromy no single set of quantum numbers or single valued action variables can be defined globally over the whole range of $\mathcal{E}M$.

6 Discussion

Following its discovery [2] monodromy became a well understood property [1] commonly found in Hamiltonian dynamical systems. Yet it and its implications in quantum mechanics remain widely unrecognized. Together with other recent studies [8,9,20,22] our example turns monodromy into a basic tool of the analysis of physical systems. For the parametric family of model integrable problems (1) monodromy exists in an open interval of the values of the parameter and thus is a stable phenomenon. It can further be suggested that monodromy and related quantum phenomena will persist after deformation to a non-integrable case.

Our example has truly numerous applications. With variations and higher order terms the Hamiltonian (1) can describe spin-rotation coupling in molecules and spin-orbit coupling in atoms in the presence of magnetic field, rotational structure of overtones of degenerate vibrational modes, vibrational structure of quasi-degenerate electronic states (Jahn-Teller effect). If the above was not enough, it also applies to *all* perturbed Kepler problems, such as atoms (without spin effects) in fields (cf. [21,4,22]). In the latter case, the phase space $S_2 \times S_2$ and the $su(2) \times su(2)$ algebra of two momenta $\mathbf{N} = \mathbf{S}$ appear as a result of Keplerian normalization (n-shell approximation). Thus the first reduced Hamiltonian for a hydrogen-like atom in parallel electric and magnetic fields [4] has the form (1) with ξ representing the effect of the non-Coulombian core potential. Our note gives the framework of the analysis of all these problems. A more complete study should also address specific features of cases $|\mathbf{N}| < |\mathbf{S}|$ (quantum problem) and $|\mathbf{N}| = |\mathbf{S}|$ (reduced phase space at $J_z = 0$).

The key point of the present note is the relation between monodromy in the parametric family of classical problems and the qualitative modification of the energy spectrum of corresponding quantum Hamiltonians. We show that (in the limit $S/N \to 0$) monodromy is related to the redistribution of energy levels between different branches of the spectrum (rather than to qualitative changes in the structure of individual branches) which occurs as the control parameter γ is varied. This opens even wider perspectives of generalization since redistribution of levels can be easily observed even relatively far from the classical limit and is a universal phenomenon not confined to problems of two coupled angular momenta. In fact redistribution will most likely occur in any one parameter family of Hamiltonians with two qualitatively different limits of "good" quantum numbers. Furthermore, the two-state model ($N \gg S = 1/2$) remains the most fundamental. Thus, the high degeneracy of our system at large S and $\gamma = 1/2$ (fig. 1, right) can be obviously decomposed into a sequence of two-state intersections by an appropriate small deformation of the Hamiltonian (1).

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