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Static and dynamical manifestations of Hamiltonian monodromy

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Abstract. The word "monodromy" means "once around a course", and it refers to changes that might occur when a system goes around some closed loop [1]. We discuss here a phenomenon whose proper name is "nontrivial monodromy of action and angle variables in a Hamiltonian system"; for the obvious reason, we just call it "Hamiltonian monodromy". In this paper we describe two manifestations of Hamiltonian monodromy: a manifestation in a time-dependent classical system, and a manifestation in a stationary quantum system. Then we give a brief description of the mathematical theory, and finally close with a short survey of previous work on this subject.

1. Monodromy in a time dependent classical system

Consider a classical particle, moving in two dimensions with coordinates (x, y) and momenta (p_x, p_y). The particle moves on a cylindrically-symmetric potential-energy barrier, and it is confined by a hard wall. Thus the Hamiltonian is

$$H(p,q) = (p_x^2 + p_y^2)/2 + V(\rho) \tag{1a}$$
$$\rho = (x^2 + y^2)^{1/2} \tag{1b}$$
$$V(\rho \le \rho_{max}) = -k\rho^2/2 \tag{1c}$$
$$V(\rho > \rho_{max}) = \infty \tag{1d}$$

In our calculations we chose $k = 2$ and $\rho_{max} = 3$. If no additional forces act upon the particle, then energy $E = H(p, q)$ and angular momentum $L = xp_y - yp_x$ are conserved. One family of solutions is given by

$$x(t; E, L) = \pm\rho_{tp}(E, L)cosh(\lambda t) \tag{2a}$$
$$y(t; E, L) = \pm\frac{L}{\mu\lambda\rho_{tp}(E, L)}sinh(\lambda t) \tag{2b}$$

where $\lambda = (k/\mu)^{1/2}$ and $\rho_{tp}(E, L)$ is the inner turning point. A typical trajectory is shown in Fig. 1.

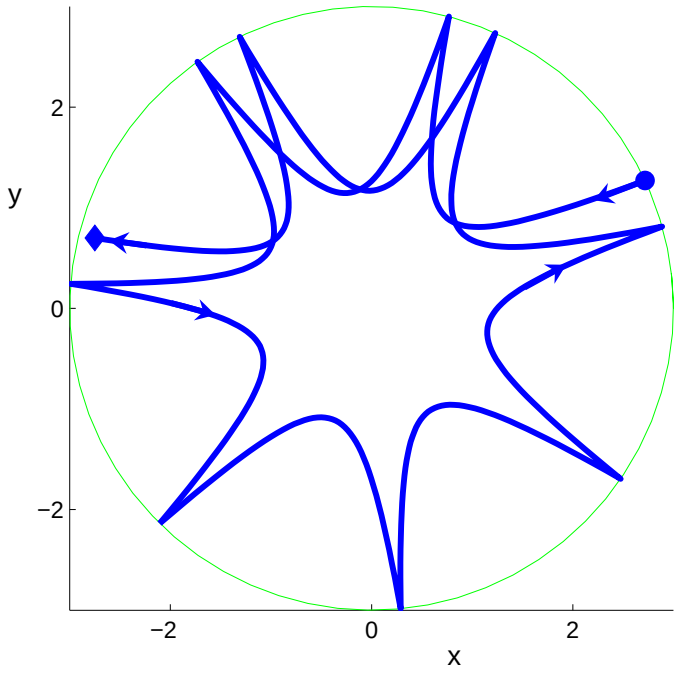

Figure 1. The blue curve traces a typical trajectory of a particle in a negative quadratic potential bounded by a circular hard wall (green line). The particle has positive angular momentum L and negative energy E (less than the maximum of the potential energy, which is located at the origin).

Now suppose there are *additional* forces and torques that change the energy and angular momentum. Suppose in particular that these additional forces drive the particle around a loop in the (L, E) plane (Fig. 2).

Movie 1 (`newmonodromy1.avi`) shows the resulting path of the particle. The blue arrow represents the location in the (L, E) plane. The green circle represents the boundary of a classically forbidden region, $\rho = \rho_{tp}(E, L)$, inside which the particle cannot enter. The particle begins at the outer turning point with energy negative and $L = 0$, so it moves initially on a straight line between the outer wall and an inner turning point at the green circle.

As $L(t)$ increases, the particle begins moving around counterclockwise. When $E(t)$ increases, the particle bounces around the enclosure in ever larger leaps. Then when $L(t)$ decreases, passing through zero with $E(t)$ positive, the particle moves on nearly a straight line, passing near the origin as the classically-forbidden region shrinks (and at one instant of time, vanishes). As $L(t)$ goes negative, the particle moves clockwise, then the angle subtended between bounces decreases. When finally $E(t)$ approaches its initial value and $L(t)$ approaches zero, the motion of the particle approaches again a straight radial line, bouncing between the hard wall and the inner turning point. Nothing about this motion is surprising.

Suppose we start two noninteracting particles at the same initial energy, both beginning at the outer wall, but displaced from each other by some angle $\Delta\phi$ (movie 2, `newmonodromy2.avi`). What is the motion of the pair? Because the system has cylindrical symmetry, the green particle remains always at the same angle $\Delta\phi$ counterclockwise from the black particle.

Now let us start two particles at the same azimuthal angle but opposite radial phase:

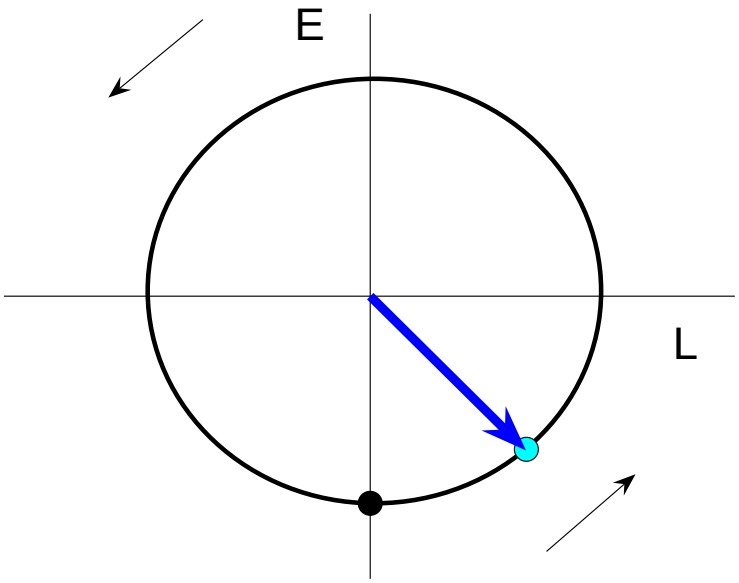

Figure 2. External forces and torques can change the energy E and angular momentum L of the particle such that their values form a closed loop encircling the origin of the (L, E) plane. That point is (in the present case) a monodromy point, and the path around it in the (L, E) plane is called a monodromy circuit.

one starts at the outer turning point and one at the inner turning point (movie 3, `newmonodromy3.avi`). They will follow different paths, but we expect that the paths will remain reasonably close. Indeed, for the first half of the movie, we see the two particles playing leapfrog with each other. However, after $L(t)$ passes through zero with $E(t)$ positive, we see that the particles are rather far apart. At the end, when $L(t)$ is again equal to zero and the energy is negative, the particles are exactly opposite each other, π apart in radial phase (as they were at the beginning) and also π apart in azimuthal angle.

Finally let us begin a family of particles, all with the same initial energy, all with $L = 0$, all starting on one radial line, but beginning with various radial phases (movie 4, `newmonodromyloop.avi`). The black one again starts at the hard wall, the red one at the inner turning point, and the blue ones in between, some with velocity inwards and some outwards. (Again the particles are noninteracting, so they can pass right through each other.) At first they oscillate on the radial line, and then as soon as the angular momentum is nonzero, we see that they form a continuous loop with a crease at the outer wall. As the paths evolve, the loop becomes ever wider. Half way around the monodromy circuit, when $L(t)$ passes through zero with $E(t)$ positive, at the instant that the classically forbidden region disappears, one of the paths on the loop passes right through the origin. After that, the necklace of particles surrounds the classically forbidden region. When we get back to negative energy and $L(t) = 0$, the initial loop has evolved into a topologically different loop.

This is a dynamical manifestation of Hamiltonian monodromy: a loop of initial conditions evolves continuously in time into a topologically different final loop, which could not be reached by any isoenergetic distortion of the initial loop.

2. Monodromy in a stationary quantum system

The time-dependent phenomenon discussed above follows from certain properties of the stationary system in the absence of additional applied forces. We discuss here a manifestation of Hamiltonian monodromy that occurs in stationary systems. It is easiest to see in a quantum system. We show in movie 5 (`regularspectrum.wmv`) and movie 6 (`monodromyspectrum.wmv`) two energy spectra of hydrogen in crossed external electric and magnetic fields. The horizontal axis is a quantum number identified by Pauli, somewhat analogous to an angular momentum, and generally called q. The vertical axis is the second-order energy shift of the levels. In movie 5, the fields are perpendicular with the magnitudes $B = 40T$, $F = 26.5kV/cm$, and the principal quantum number $n = 7$. We see that the energy levels lie on a regular lattice. Although it is hardly necessary to do so, the regularity of this lattice is emphasized by transporting a pair of lattice vectors around a closed loop. The vectors return to themselves.

In contrast, at different field ratios the spectrum may have a defect. The spectrum shown in movie 6 has a lattice defect. (In this case $B = 0.302T$, $F = 175V/cm$, $n = 15$ and again the fields are precisely perpendicular.) Near the center of the picture is a cyan diamond. (This point is analogous to the point$(L = 0, E = 0)$ in the previous section, around which we transported the classical system.) In the quantum spectrum, this point is the source of a lattice defect. Transporting a pair of lattice vectors smoothly around the cyan diamond, we see that the horizontal arrow does not return to itself. This is a quantum manifestation of Hamiltonian monodromy.

3. A bit of mathematical theory

Above we discussed two very different phenomena in two very different systems. It is not at all obvious that these phenomena are related. In fact, however, they are two manifestations of "nontrivial monodromy of action and angle variables in Hamiltonian systems". Let us give a brief explanation of what this means.

Consider a bound classical system with two degrees of freedom, having coordinates and momenta $(\mathbf{r}, \mathbf{p})$. If there exists an independent function $Q(\mathbf{r}, \mathbf{p})$ whose Poisson bracket with the Hamiltonian $H(\mathbf{r}, \mathbf{p})$ vanishes, $[Q(\mathbf{r}, \mathbf{p}), H(\mathbf{r}, \mathbf{p})] = 0$ then trajectories lie on two-dimensional tori in the four-dimensional phase space, and these tori are connected components of level sets of $Q(\mathbf{r}, \mathbf{p})$ and $H(\mathbf{r}, \mathbf{p})$,

$$Q(\mathbf{r}, \mathbf{p}) = q \tag{3a}$$
$$H(\mathbf{r}, \mathbf{p}) = h \tag{3b}$$

where q and h are constant numerical values. In this case, action variables can be constructed, and these actions may be regarded as functions of $(\mathbf{r}, \mathbf{p})$ or of (q, h).

$$\tilde{J}(\mathbf{r}, \mathbf{p}) = J(q, h) \tag{4}$$

The latter function $J(q, h)$ can be constructed from a differential form,

$$dJ = T(q, h)dh + \Theta(q, h)dq \tag{5}$$

From general properties of Hamiltonian flow, it can be shown that this differential form is closed − cross derivatives are equal:

$$\frac{\partial T(q, h)}{\partial q} = -\frac{\partial \Theta(q, h)}{\partial h} \tag{6}$$

If the functions $Q(\mathbf{r},\mathbf{p})$ and $H(\mathbf{r},\mathbf{p})$ are independent and the functions $T(q,h)$ and $\Theta(q,h)$ are single-valued and satisfy Eq. (6) over a simply-connected region of the (q,h) plane, then integration of Eq. (5) gives the function $J(q,h)$.

In Hamiltonian systems having monodromy, some of the above assumptions fail. First, for certain values of $(\mathbf{r},\mathbf{p})$, $Q(\mathbf{r},\mathbf{p})$ and $H(\mathbf{r},\mathbf{p})$ might not be independent. For example, if $(\mathbf{r},\mathbf{p}) = (x, y, p_x, p_y)$, and

$$H(\mathbf{r},\mathbf{p}) = \mathbf{p}^2/2 - \mathbf{r}^2/2 \tag{7a}$$

$$Q(\mathbf{r},\mathbf{p}) = \mathbf{r} \times \mathbf{p} \tag{7b}$$

then at $(\mathbf{r} = \mathbf{0}, \mathbf{p} = \mathbf{0})$, the phase space gradients of both $Q(\mathbf{r},\mathbf{p})$ and $H(\mathbf{r},\mathbf{p})$ vanish, so in that vicinity, the functions are not independent. We say that $(\mathbf{r} = \mathbf{0}, \mathbf{p} = \mathbf{0})$ is a singular point in phase space, and the corresponding value $(q = 0, h = 0)$ is a singular value in the (q,h) plane, which we call a monodromy point.

Second, in some cases $\Theta(q,h)$ may represent a geometrical angle that changes by 2π upon traversing a circuit around the monodromy point in the (q,h) plane. This happens for example in the barrier system, for which $\Theta(q,h)$ is the angle subtended between bounces.

In such cases, the differential form, Eq. (5), is closed but not exact in the plane (excluding the origin). Integration of this differential form produces a "function" that is multivalued, and has multivalued derivatives. A picture of such a multivalued action is shown in Fig. 3.

From this, we can understand the defect in the quantum lattice. Quantum eigenvalues can be calculated to good approximation from quantized values of action variables. For hydrogen in weak crossed fields, one of three action variables corresponds to the principal quantum number n, which is held fixed in movies 5 and 6. Averaging over the corresponding angle variable (i.e. averaging over a Kepler ellipse) reduces the system to two degrees of freedom. A second action variable is a function called Q , which is quantized as $Q = integer$. Thus in the plane, all numerically computed quantum eigenvalues lie very close to vertical lines spaced by integers. The third action variable is the multivalued function shown in Fig. 3. Contours of one continuous sheet of that function are shown in Fig. 4. The arrows show what happens to contours of that function when we traverse a monodromy circuit (a closed path around the monodromy point). It follows that the lattice of quantum eigenvalues has a defect.

If an action $J(q,h)$ is a multivalued function of (q,h), it follows that an angle must also be multivalued. Let $J_k^{initial}$ and J_k^{final} be initial and final action variables on a monodromy circuit. In the cases considered here, they are related in the following way:

$$J_1^{final} = J_1^{initial} \tag{8a}$$

$$J_2^{final} = J_2^{initial} - M J_1^{initial} \tag{8b}$$

where $M = 2$ for hydrogen (at these fields) and $M = 1$ for the barrier system. Canonically conjugate angles (ϕ_1, ϕ_2) must be related by

$$\phi_1^{final} = \phi_1^{initial} + M\phi_2^{initial} \tag{9a}$$

$$\phi_2^{final} = \phi_2^{initial} \tag{9b}$$

This fact leads to consequences in a time-dependent system. In the barrier system, it is possible to "realize" a monodromy circuit by applying additional forces and torques. We may begin with a family of phase-space points that forms one fundamental loop on the initial torus

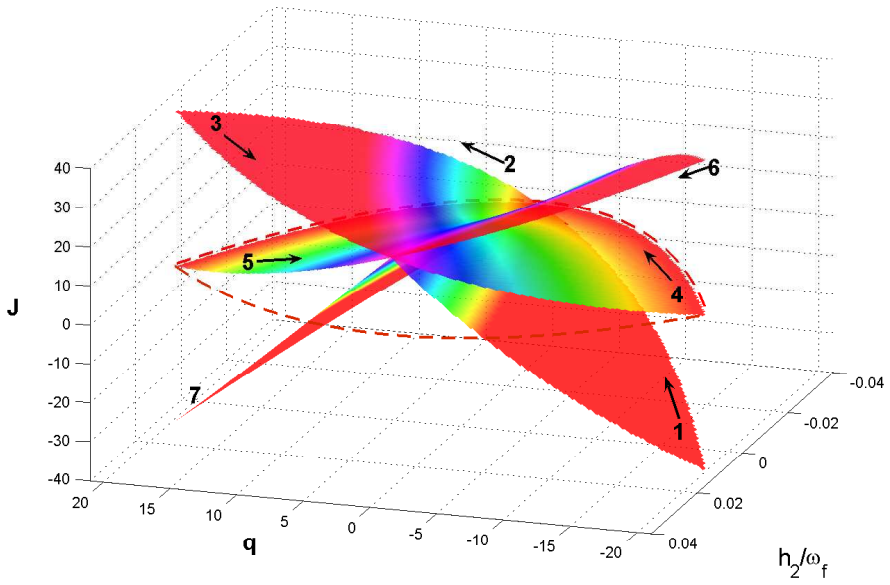

Figure 3. For some field strength ratios, Hydrogen in crossed fields has an intrinsically multivalued action variable $J(q, h_2)$ (here, $\mathbf{F} \cdot \mathbf{B} = 0$ $n = 20$, $tan^{-1}[3nF/B] = 50^o$ and $\omega_f = \sqrt{B^2 + (3nF)^2}/2 << 1/n^3$). The set of all values of the constants of the motion q and h_2 which are classically allowed at fixed $n = 20$ are contained within the dashed red boundary. Inside this boundary there is one point where J is not defined, at $q = 0$ and $h_2 \sim 0.01\omega_f$ (the monodromy center). Away from this point, J is locally smooth everywhere only if it is multivalued, with a branch point at the monodromy center. Three branches of the function are plotted in the figure. To continue the classical action variable smoothly, we may start at (1) and follow the arrows sequentially along the surface all the way to (7); then we pass onto a new branch every time we cross $q = 0$ if h_2 is above the monodromy center.

$0 \leq \phi_1 < 2\pi$. In an ideal case, every trajectory begins on one torus $(q(0), h(0))$, and additional disturbances are applied such that all trajectories evolve smoothly and synchronously to other tori $(q(t), h(t))$. Also, ideally, each angle variable may evolve such that

$$\phi_k(t) = \phi_k(0) + \int_0^t \omega_k(q(t'), h(t'))dt' \tag{10a}$$

$$\omega_k = \left(\frac{\partial H}{\partial J_k}\right)_{\mathbf{J}(t)} \tag{10b}$$

In this ideal case, all actions and angles evolve synchronously, following the variables on the instantaneous tori. Then if $(q(t), h(t))$ undergo a circuit around the monodromy point, the static variables change character: one fundamental loop becomes a different loop according to Eq. (9a).

In exactly the same way, on the actual paths followed in real time by the family of particles, the initial loop evolves continuously in time to a topologically different loop.

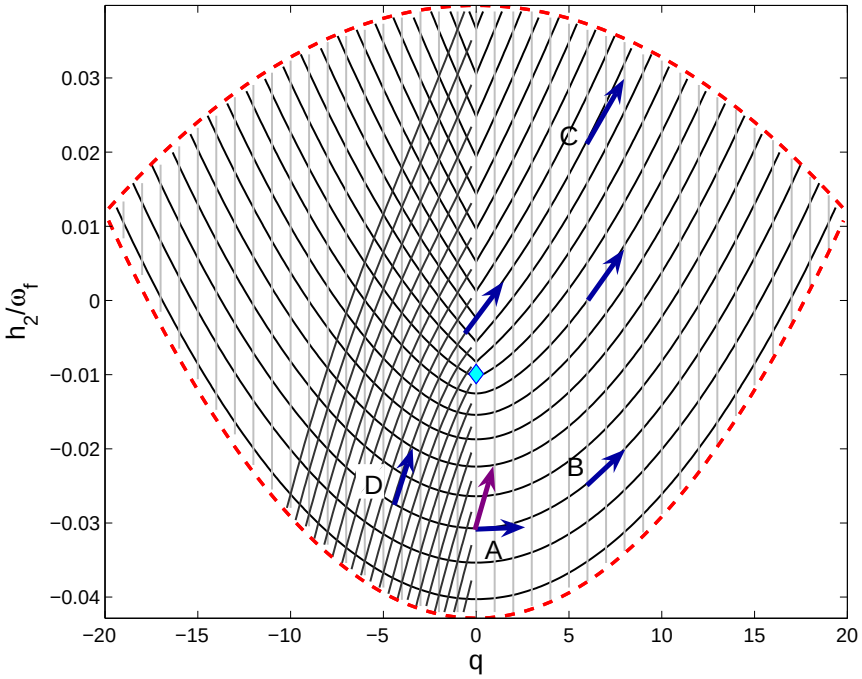

Figure 4. Contours of a multivalued classical action variable $J(q, h_2)$ for Hydrogen in crossed fields ($\mathbf{F} \cdot \mathbf{B} = 0$ $n = 20$ and $tan^{-1}[3nF/B] = 50^o$). The contours of the principal branch J are shown in the entire spectrum, while some contours of a second branch are shown for $q < 0$. At (A) the blue vector is tangent to contours of the principal branch of J. From (A) this vector is transported along the contours of J to (B), then along contours of q to (C), then along contours of J to $q = 0$ where the contours of J do not pass smoothly through $q = 0$. To obtain a smooth classical action variable the principal branch must be continued across $q = 0$ to the function $J^{cont} = J - 2q$. Along contours of J^{cont} the vector is transported down to (D). When the blue vector is transported along contours of the original sheet to return to (A), the original blue arrow has rotated into the purple arrow.

4. A brief history

In all the above, we stated results without giving proper credit to those who developed this subject. Let us now give a very brief history. The existence of nontrivial monodromy of action and angle variables was first recognized by Duistermaat [2]. He showed that under certain conditions, when we traverse a monodromy circuit, smoothly connecting angle coordinates on each torus to those on adjacent tori, then when we return to the initial torus, the final angle coordinates do not match the initial ones. Cushman was quick to recognize that there are many physical systems having this type of monodromy; the spherical pendulum and the Lagrange top are discussed in his book with Bates [3]. Cushman and Duistermaat [4] soon realized that monodromy of action variables would have implications for a quantum system, and they were the first to show the rotation of lattice vectors.

Bates [5] pointed out that a simple system having monodromy is the cylindrically symmetric smooth barrier $V(\rho) = -k\rho^2/2 + a\rho^4$ (called the "Champagne bottle" in Europe, or the "Mexican hat" in the US), and Child [6] discussed the quantum implications. (The barrier system discussed in the present paper incorporates a hard outer wall instead of the quartic term; the advantage

is that all integrals are elementary.)

Starting about 1999, a number of groups recognized that many important molecular systems display quantum monodromy: systems with coupled angular momenta were studied by Sadovskii and Zhilinskii [7], oriented polar molecules were studied by Kozin and Roberts and by Arango et al. [8], the water molecule was studied by Tennyson and collaborators [9], the CO_2 molecule by Cushman et al. [10], and a collection of quasilinear molecules was studied by the Winnewisser team [11]. Monodromy also shows up in ellipsoidal billiards and in the two-center problem, as was shown by Waalkins, Dullin and Junge [12].

The study of the spectrum of hydrogen in crossed fields also has a long history, going back to Pauli [13], who discussed the spectrum to first order in the fields. The second-order spectrum was studied by Solove'v [14], Braun [15], and Uzer and his collaborators [16]. Sadovskii and Cushman [17] were the first to recognize that the second order spectrum of hydrogen in perpendicular fields has monodromy (in a certain range of field strengths). Later Schleif [18] calculated the spectrum in near-perpendicular fields, and showed that the monodromy point with $M = 2$ splits into two monodromy points having $M = 1$ in a certain range of field strengths, and that other more complicated structures appear at other field strengths; then additional classical calculations were made by Efstathiou et al [19].

Our group seems to be the first to point out that the above static manifestations of monodromy imply that there must also be dynamical manifestations, and this paper might turn out to be the first published account [20]. When additional forces are applied to a Hamiltonian system having monodromy, we saw in movie 4 that a family of noninteracting particles, or a family of trajectories, can display the same surprising topological change that is present in the angle variables. A number of papers discussing this in detail are in preparation or have been submitted [21].

Acknowledgments

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References

[1] In complex variable theory a monodromy theorem states that if a complex variable z is taken around a closed path in the complex plane, then a function f(z) returns to its original value provided that the function has no branch points in the region enclosed by that path. (Weisstein, Eric W. "Monodromy Theorem." From MathWorld, `http://mathworld.wolfram.com/MonodromyTheorem.html`.) In classical dynamics a monodromy matrix associated with a periodic orbit describes the relationship between initial displacements and final displacements from a periodic orbit: in the linear approximation the vector of final displacements is equal to the monodromy matrix times the vector of initial displacements.

[2] Duistermaat J J 1980 *Comm. Pure Appl. Math.* **33** 687

[3] Bates L M and Cushman R H 1997 *Global aspects of classical integrable systems* (Basel: Birkhauser)
Another book describing a number of classical systems in amodern perspective is:
Efstathiou K 2004 *Metamorphoses of Hamiltonian systems with symmetries* (Berlin: Springer)

[4] Cushmann R H and Duistermaat J J 1988 *Bull. Am. Math. Soc.* **19** 475
Further mathematical developments on Quantum Monodromy are given by:
Vu Ngoc S 1999 *Commun. Math. Phys.* **203** 465-479
Vu Ngoc S 2000 *Commun. Pure Appl. Math. Phys.* **53** 143-217

[5] Bates L M 1991 *J. Appl. Math. Phys.* **42** 837

[6] Child M S 1998 *J. Phys. A: Math. Gen.* **31** 657-670

[7] Sadovskii D A and Zhilinskii B I 1999 *Physics Letters A* **256** 235

[8] Kozin I N and Roberts R M 2003 *J. Chem. Phys.* **118** 10523
Arango C A, Kennerly W W and Ezra G S 2004 *Chem. Phys. Lett.* **392** 486
Arango C A, Kennerly W W and Ezra G S 2005 *J. Chem. Phys* **122** 184303

[9] Child M S, Weston T and Tennyson J 1999 *Mol. Phys.* **96** 371

Zobov N F, Shirin S V, Polyansky O L, Tennyson J, Coheur P F, Bernath P F, Carleer M and Colin R 2005 *Chem. Phys. Lett.* **414** 193.
[10] Cushman R H, Dullin H R, Giacobbe A, Holm D D, Joyeux M, Lynch P, Sadovski D A, Zhilinski B I 2004 *Phys. Rev. Lett.* **93** 024302
Giacobbe A, Cushman R H, Sadovski D A and Zhilinski B I 2004 *J. Math. Phys.* **45** 5076
[11] Winnewisser B P, Winnewisser M, Medvedev I R, Behnke M, De Lucia F C, Ross S C, and Koput J 2005 *Phys. Rev. Lett.* **95** 243002
Winnewisser M, Winnewisser B P, Medvedev I R, De Lucia F C, Ross S C, Bates L M 2006 *Journal of molecular structure* **798** (no. 1) 1
[12] Waalkens H and Dullin H R 2002 *Annals of Physics* **295** 81-112
[13] Pauli W 1926 *Z. Phys.* **36** 336
English Translation: Van der Waerden B L 1967 *Sources of Quantum Mechanics* (New York: Dover)
[14] Solove'v E A 1983 *Sov. Phys. JETP* **58** 63
[15] Braun P A 1993 *Rev. Mod. Phys.* **65** 115
[16] Gourlay M J, Uzer T and Farrelly D 1993 *Phys. Rev. A* **47** 3113
Milczewski J and Uzer T 1997 *Phys. Rev. A* **56** 220
[17] Cushman R H and Sadovski D A 1999 *Europhys. Lett.* **47** 1
Cushman R H and Sadovski D A 2000 *Physica D* **142** 166
[18] Schleif C R and Delos J B 2007 *Phys. Rev. A* **76** 013404
[19] Efstathiou K, Sadovski D A and Zhilinski B I 2007 *Proc. Roy. Soc. Ser. A* **463** 1771
[20] Despite our best efforts.
[21] Delos J B, Dhont G D, Sadovski D A and Zhilinski B I *Dynamical manifestations of Hamiltonian monodromy* (submitted)