NORMAL FORMS, GEOMETRY, AND DYNAMICS OF ATOMIC AND MOLECULAR SYSTEMS WITH SYMMETRY

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We show how general ideas of Louis Michel on the application of topology, group theory, and commutative algebra in the qualitative analysis of symmetric dynamical systems can be concretized for finite-dimensional Hamiltonian dynamical systems with symmetries, notably atoms and molecules. This talk is a contribution to the special session in the memory of *Louis Michel*.

1 Introduction

In his work Louis Michel was always determined to extract as much information as possible from the symmetry and topology of the physical systems he studied; he used to call his approach as a program of *Symmetry and Topology*. His collaboration with Boris Zhilinskií on the application of this general program to atomic and molecular systems resulted in a development of the method of qualitative analysis, a set of concrete mathematical tools, based on group theory, basic topology, Morse theory, commutative algebra, and invariant theory. We show on a number of concrete examples of real molecular and atomic systems, which represent the class of finite dimensional Hamiltonian dynamical systems with symmetries, how this method is implemented. A general review of the qualitative analysis can be found in Chapters I-III of [I]; our dynamical analysis, in particular the use of invariants for reduction (and singular reduction) of symmetries was greatly influenced by Richard Cushman.[II] We restricted the rest of the bibliography to our papers whose results were used in the talk; these papers should be looked up for the references to the related work by other authors.

2 Tools for qualitative and dynamical analysis

We give a brief summary of the stages of the qualitative and dynamical analysis of atomic and molecular systems.[I]

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We formulate the problem and study the symmetry group G of our system, typically a finite group which includes geometric and time-reversal operations. In certain cases we consider (construct) a classical analogue of a given quantum system. Otherwise, when the classical initial system is known *a priori*, we propose the *dynamical symmetry*, typically an approximate continuous S_1 symmetry, and the way to reduce this classical system. If the strict symmetry of the system G has continuous elements, we consider reduction of such symmetries as well. In all cases we end up studying a reduced classical Hamiltonian system defined, normally, over a compact reduced phase space P. We further study the topology of P, in particular we look for the Betty numbers of P.

We describe the action of the initial symmetry group G on the reduced phase space P. We use polynomial invariants of the dynamical symmetry as coordinates on P. We further symmetrize these invariants with respect to G and use them to describe the action of G on P. We construct the *orbit space* $\mathcal{O}$ of this action and consider the stratification of P. We find fixed points (*critical orbits*) and invariant subspaces of the group action.

We further study the commutative algebra of our invariants and the structure of the ring of all polynomial invariants. We find the *integrity basis*, which is a more sophisticated variety of the Gröbner basis and which allows to represent unambiguously any polynomial in this ring and therefore any analytic function on P in terms of invariants. Explicit construction of the integrity basis is greatly facilitated by the *Molien generating function* which we compute for the given group action on invariant polynomials.

We assume that our reduced Hamiltonian is in the class of simplest Morse functions on P. Such functions have the minimum number of stationary points compatible with topology and symmetry. These points are *relative equilibria* of the system. Points in the critical orbits of the group action are necessarily stationary, points in the same orbit are equivalent. Further restrictions on the stability of stationary points are imposed by their local symmetry (stabilizer). Taking all this into account we place stationary points on the critical orbits and check if the Morse inequalities and Euler equation for P are satisfied. Normally this singles out a few possible minimum sets of stationary points; it may occur, however, that additional stationary points must be placed on non-critical orbits in order to satisfy Morse theory. These latter points are also relative equilibria but their exact position on P depends on the concrete Hamiltonian.

We construct parametric families of simplest polynomial Morse Hamil-

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tonians $\mathcal{H}$ from the integrity basis invariants. Such Hamiltonians are of the lowest degree which is sufficient to represent correctly the simplest G-invariant Morse function on P; they typically have a small number of parameters. We study $\mathcal{H}$ as a function on the orbit space $\mathcal{O}$. We classify constant level sets $\{\mathcal{H} = h\}$ of different $\mathcal{H}$ on $\mathcal{O}$. Geometrically we look for intersections of the surface $\mathcal{H} =$ const and the orbifold $\mathcal{O}$, both defined in invariant polynomial coordinates[a]. Relative equilibria (stationary points) of different kinds correspond to exceptional sections $\{\mathcal{H} = h\} \cap \mathcal{O}$ We find the energies of relative equilibria, i.e., the values h of $\mathcal{H}$ at such sections. Our qualitative analysis reaches its destination: each $\mathcal{H}$ is represented entirely by the family of its level sets on $\mathcal{O}$. We also consider bifurcations which lead to qualitatively different families of constant level sets and which occur when parameters of $\mathcal{H}$ are made to vary.

We transfer our results to quantum mechanics. We use energies of relative equilibria to define energy limits for the multiplets of quantum states. We predict localization patterns near stable relative equilibria, and corresponding regular sequences of levels. Finally we study quantum analogues of $\mathcal{H}$.

2.2 Analytical and dynamical analysis

The two important complements to the general scheme of Michel and Zhilinskií are based on the normalization (analytical aspect) and the Poisson structure of the reduced system (dynamical aspect). We normalize the initial classical Hamiltonian H explicitly in order to reduce the dynamical symmetry, the truncated normal form $H_{\text{n.f.}}$ is expressed in terms of dynamical invariants using integrity basis. The invariant which represents the approximate dynamical integral of motion is replaced by its value and becomes a parameter. This makes $H_{\text{n.f.}}$ a *reduced Hamiltonian* H_{red} on the reduced phase space P. We can also consider H_{red} as a function on the orbit space $\mathcal{O}$.

We study relative equilibria of H_{red} analytically, in particular we verify whether H_{red} is of the simplest Morse type. We consider H_{red} as a parametric family and look for bifurcations of relative equilibria, or, more generally, of constant level sets of H_{red} on $\mathcal{O}$. We reconstruct relative equilibria as periodic orbits of the original classical mechanical system. Furthermore, we reconstruct the entire geometry of (the integrable approximation to) the original system, i.e., we reconstruct all dynamically invariant subspaces of this system (invariant KAM tori) and describe how these subspaces fit together and foliate the constant energy level set of the initial phase space. We now can do full EBK quantization.

[a] This method of sections is also widely used by R. Cushman.

We equip the commutative algebra of the generators of the ring of invariant polynomials with a Poisson structure by appropriately restricting the Poisson brackets of generators. The latter become dynamical variables of the reduced system and we write Euler–Poisson equations of motion on the reduced phase space P. Though not general, this simple method works in all cases we discuss. We can further restrict these equations to invariant subspaces of P.

3 Hénon-Heiles system: an illustration

We follow the scheme of the qualitative analysis on the example of the well known model system, the three-fold symmetric perturbation of the 1:1 harmonic oscillator. The initial Hénon-Heiles Hamiltonian

$$H = H_0 + \epsilon V(q) = \frac{1}{2}(p_x^2 + q_x^2) + \frac{1}{2}(p_y^2 + q_y^2) + \epsilon \left(\frac{1}{3} q_x^3 - q_x q_y^2 \right) \qquad (1)$$

is a function on R_4 with standard symplectic structure $q_x \wedge p_x + q_y \wedge p_y$. The spatial symmetry group of (1) is a dihedral group D_3, the full symmetry group is $D_3 \times \mathcal{T}$ where $\mathcal{T}$ is a Z_2 symmetry of the kind $(q, p) \to (q, -p)$ often called *time reversal* or *momentum reversal*.

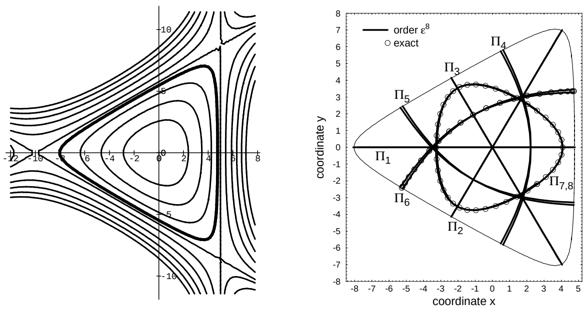

Figure 1. Hénon-Heiles potential $V(q)$ calculated for $\epsilon = 0.1$ and $E/E_{\mathrm{saddle}} = 0.2, 0.45, 0.7, \mathbf{0.9}, 1, 1.2, \ldots$ (left); Relative equilibria (nonlinear normal modes) of the Hénon-Heiles system reconstructed from the ϵ^8 normal form at the energy $E/E_{\mathrm{saddle}} = 0.9$ (right).

3.1 *Dynamical symmetry, invariants, reduced phase space*

The dynamical S_1 symmetry is generated by the flow of the unperturbed 1:1 oscillator. Using variables $z = q + ip$ we can write the four quadratic invariants of this symmetry as follows

$$H_0 = 2J = \frac{1}{2}(z_x\bar{z}_x + z_y\bar{z}_y), \quad \mathbf{J} = \begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix} = \frac{1}{4}\begin{pmatrix} z_x\bar{z}_y + z_y\bar{z}_x \\ iz_x\bar{z}_y - iz_y\bar{z}_x \\ z_x\bar{z}_x - z_y\bar{z}_y \end{pmatrix}. \tag{2}$$

The Poisson algebra generated by the components of the 3-vector $\mathbf{J}$ is the standard so(3) with bracket $\{J_a, J_b\} = \epsilon_{abc}J_c$ and Casimir $J = |\mathbf{J}|$ (or H_0). For each constant value of the dynamical integral J we construct the reduced phase space P^J as a 2-sphere S_2^J embedded in the ambient space R_3 with coordinates (J_1, J_2, J_3). The defining equation of P^J is, of course,

$$J^2 = J_1^2 + J_2^2 + J_3^2 = \text{const}, \tag{3}$$

which is also the only algebraic relation between (J_1, J_2, J_3).

3.2 Group action, critical orbits, and stationary points

The action of the symmetry group $D_3 \times \mathcal{T}$ on S_2^J is equivalent to the action of the point group D_{3h} of transformations of the R_3 space[b] which acts naturally on $S_2^J \subset R_3$. Since J_2 is invariant with respect to any rotation of the initial coordinates (x, y), it is convenient to choose J_2 along the vertical axis. Then time reversal $\mathcal{T}$ acts as the horizontal reflection plane $(J_1, J_2, J_3) \to (J_1, -J_2, J_3)$. The action of $D_3 \times \mathcal{T}$ has 8 fixed points which form three critical orbits characterized in table 1.

Table 1. Critical orbits of the $D_3 \times \mathcal{T} \sim D_{3h}$ action on the reduced phase space S_2^J of the Hénon-Heiles system. The $C_3 \wedge \mathcal{T}_2$ subgroup of $D_3 \times \mathcal{T}$ is generated by C_3 and $\mathcal{T}_2 = C_2 \circ \mathcal{T}$; the groups $C_3 \wedge \mathcal{T}_2$, D_3, and C_{3v} are isomorphic as abstract groups. "Historic" labels Π_k of the were introduced for the nonlinear normal modes by Montaldi, Roberts and Stewart and used later in [2]. Note that $(J_1, J_2, J_3) = J(\sin\theta\sin\varphi, \cos\theta, \sin\theta\cos\varphi)$.

orbit	stabilizer	ξ/J^3	μ/J^2	θ	φ
$\Pi_{7,8}$	$C_3 \wedge \mathcal{T}_2$	0	1	0	–
$\Pi_{4,5,6}$	$C_2 \times \mathcal{T}$	$-1/2$	0	$\pi/2$	$0,\ \pm 2\pi/3$
$\Pi_{1,2,3}$	$C_2' \times \mathcal{T}$	$1/2$	0	$\pi/2$	$\pi,\ \pm\pi/3$

The simplest D_{3h} invariant Morse function $\mathcal{H}$ on S_2 has eight stationary points which are situated on the critical orbits described in table 1. These

[b]We use Schönflis notation for point groups, see M. Hamermesh, *Group theory and its application to physical problems* (Addison-Wesley, Reading, 1964).

points should satisfy the Euler relation for the sphere S_2

$$c_0 - c_1 + c_2 = 2,$$

where c_0, c_1, and c_2 are the numbers of maxima, saddle points, and minima. Furthermore, since the two equivalent $\Pi_{7,8}$ points on S_2 have the stabilizer C_3, the three-fold rotation symmetry, these points should be elliptic (stable). Of the two three-point orbits with stabilizers C_2 and C_2', one should accommodate elliptic points and the other—hyperbolic (unstable). One possible simplest Morse function is drawn in fig. 2, left. It has two equivalent maxima at $\Pi_{7,8}$, three equivalent minima at $\Pi_{1,2,3}$ and three equivalent saddle points at $\Pi_{4,5,6}$.

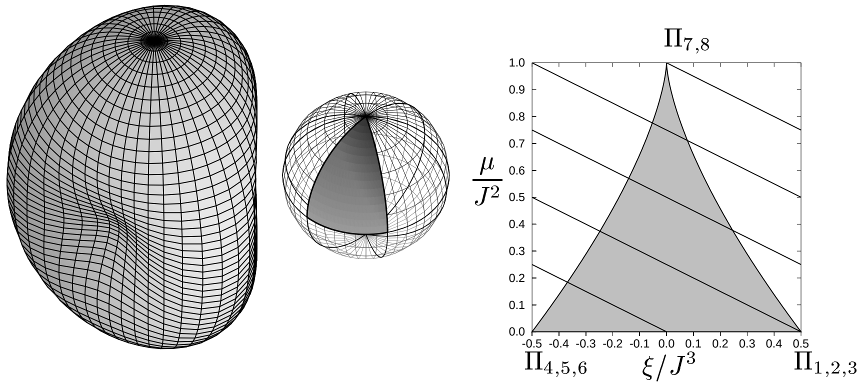

Figure 2. Relative equilibria of the Hénon-Heiles system as stationary points of the reduced Hamiltonian $H^J_{\mathrm{n.f.}}$ on the reduced phase space S^J_2. On the left we show $H^J_{\mathrm{n.f.}}$ as a function on S^J_2. The shaded area on the right and central panel represents the orbit space (orbifold) $\mathcal{O}$ of the $D_3 \times \mathcal{T}$ action on S_2; straight lines in the right panel are constant level sets of the simplest $D_3 \times \mathcal{T}$-invariant Morse Hamiltonian $\mathcal{H} = \mu + \epsilon\xi$.

3.3 Integrity basis

The generating function for the polynomials in four initial phase space variables $(z_x, z_y, \bar{z}_x, \bar{z}_y)$ invariant with respect to the S_1 symmetry of the harmonic oscillator

$$g(\lambda) = (1 + \lambda^2)/(1 - \lambda^2)^3, \tag{4}$$

where the formal variable λ represents any $(z, \bar{z})$, is computed directly from the Molien theorem.[11] The ring $\mathcal{R}$ of invariant polynomials generated by (J_1, J_2, J_3) is not free because of the algebraic relation (3). We can decompose this ring as $\mathcal{P}(J, J_1, J_2) \cdot \{1, J_3\}$ meaning that any member in $\mathcal{R}$ can be expressed using terms $J^a J_1^b J_2^c$ and $J^a J_1^b J_2^c J_3$ with (a, b, c) arbitrary nonzero integers. For instance, any power of J_3 can be represented this way using (3). The structure of $\mathcal{R}$ is confirmed by the Molien function (4) which tells that there are three *principal* or *denominator invariants* in $\mathcal{P}$ and one nontrivial *auxiliary* or *numerator invariant* in $\{\}$, all of degree 2 in $(z, \bar{z})$. This kind of information is invaluable in higher dimensional situations.

The group $D_3 \times \mathcal{T}$ acts on (J_3, J_1, J_2) in the same way as D_{3h} acts on (x, y, z), the polynomials (J_3, J_1, J_2) span the $E \oplus A_2$ representation of this group. The Molien generating function for $D_3 \times \mathcal{T}$ invariant polynomials in (J_1, J_2, J_3)

$$g(E \oplus A_2 \to A_1; \lambda) = \frac{1}{(1-\lambda^2)(1-\lambda^3)}$$

can be obtained straightforwardly from the action of the finite group $D_3 \times \mathcal{T}$ on (J_1, J_2, J_3). We conclude that the ring of all polynomial invariants of the combined action of $D_3 \times \mathcal{T}$ and oscillator symmetry S_1 is freely generated by (n, μ, ξ) where $n = 2J$ is the main oscillator invariant [see (2)] and μ and ξ are polynomials in (J_1, J_2, J_3) of degree 2 and 3 respectively. The generators can be chosen explicitly as follows

$$n = 2J, \quad \mu = J_2^2, \quad \xi = \frac{1}{2} J_3 (3J_1^2 - J_3^2). \tag{5}$$

In simple terms this means that the normalized Hénon-Heiles Hamiltonian is a function $H_{\text{n.f.}}(n, \mu, \xi)$ with n later relegated as a parameter. To our knowledge, this result of the application of elementary invariant theory has been not appreciated by the numerous studies of the Hénon-Heiles system.

3.4 Orbit space of the $D_3 \times \mathcal{T}$ action on S_2

As shown in fig. 2, right, the orbit space $\mathcal{O}$ of the $D_3 \times \mathcal{T}$ action on S_2 can be defined as an algebraic variety in the 2-plane with coordinates (μ, ξ)

$$0 \le \frac{\mu}{J^2} \le 1 - t^2, \quad \frac{|\xi|}{J^3} \le \frac{1}{2} t^3, \quad t \in [0, 1].$$

Knowing the D_{3h} action on S_2 (fig. 2, centre) we can see that $\mathcal{O}$ is the image of the triangular petal on S_2 cut out by three symmetry planes, two vertical planes intersecting at the angle $\pi/3$ and the horizontal plane. Those who prefer using algebra will consider

$$\det \left[\frac{\partial(\mu, \xi, J)}{\partial(J_1, J_2, J_3)} \right] = -6 J_1 J_2 (3J_3^2 - J_1^2) = 0$$

and observe that the borders and singular points of $\mathcal{O}$ (one- and zero-dimensional strata on S_2) correspond to simple and double zeroes of this Jacobian.

3.5 Simplest polynomial Morse Hamiltonian

Since the invariant μ has high axial symmetry S_1, the simplest polynomial Hamiltonian $\mathcal{H}$ should include the higher degree term ξ in order to have correct symmetry $D_3 \times \mathcal{T}$. Generally, at least when J is low, we expect the contribution by ξ which has higher degree in (J_1, J_2, J_3) to be less important than that of μ. The function $\mathcal{H} = a\mu + b\xi$ with $a \gg b$ is illustrated in fig. 2, left. This function is of the simplest Morse type. The family of constant level sets of $\mathcal{H}$ on the orbifold $\mathcal{O}$ has three exceptional (critical) levels which pass at $\Pi_{1,2,3}$, $\Pi_{4,5,6}$, and $\Pi_{7,8}$ (see fig. 2). The extremal levels correspond necessarily to stable relative equilibria, the critical level at the intermediate energy $\mathcal{H}_{\Pi_{4,5,6}}$ contains unstable relative equilibria and their stable/unstable manifold (separatrix). Stability of the stationary points Π of $\mathcal{H}$ is given by the frequency ω of small oscillations about them, i.e, by the coefficient in the linearization of $\mathcal{H}$ near Π. Frequencies $\omega_{\Pi_{7,8}}$ and $\omega_{\Pi_{1,2,3}}$ are defined primarily by μ and ξ contributions respectively. If $\mathcal{H} = \mu + \epsilon\xi$, $\epsilon \ll 1$, and n is small, then $\omega_{\Pi_{7,8}} \gg \omega_{\Pi_{1,2,3}}$, i.e., the $\Pi_{7,8}$ maximum is much "deeper" than $\Pi_{1,2,3}$, cf. fig. 2.

3.6 Qualitative reconstruction of relative equilibria

Stationary points of $\mathcal{H}$ are relative equilibria of the system. They correspond to special periodic orbits of the system (see fig. 1, right), which we also call nonlinear normal modes (nnm). Stability and symmetry properties of these periodic orbits is defined by stability ω and local symmetry (stabilizer) of relative equilibria. The two elliptic nnm's $\Pi_{7,8}$ are not $\mathcal{T}$-invariant and form loops in the configuration plane with coordinates (x, y). These nnm's share the same D_3 symmetric image in this plane and they run in opposite directions so that the time reversal $\mathcal{T}$ sends $\Pi_7 \leftrightarrow \Pi_8$. Periodic orbits with stabilizer $C_2 \times \mathcal{T}$ or $C_2' \times \mathcal{T}$ are $\mathcal{T}$-invariant and their (x, y) image is a line with ends connecting to the border of the allowed coordinate domain (where kinetic energy is zero) at a right angle. Since the (x, y) image is also C_2-invariant, three such nnm's lie on the C_2 axes, and three others cross these axes at a right angle. We should mention that the above qualitative description of relative equilibria was first obtained on the basis of a different approach by Montaldi, Roberts, and Stewart in 1988.

Qualitative reconstruction of invariant manifolds of (the integrable approximation to) the Hénon-Heiles system starts with the level sets $\{\mathcal{H} = h\} \cap \mathcal{O}$ (fig. 2) which should be first brought up to the reduce phase space S_2. This can be quickly done using a bit of geometric intuition. Regular sets Γ with energies $H_{\Pi_{4,5,6}} < h_\Gamma < H_{\Pi_{7,8}}$ map to two equivalent circular periodic orbits on S_2 (one goes around Π_8 and another—around Π_7), while sets Γ' with energies $H_{\Pi_{1,2,3}} < h_{\Gamma'} < H_{\Pi_{4,5,6}}$ become three equivalent periodic orbits on S_2 (each going around one of the points $\Pi_{1,2,3}$). To understand how these circular orbits fit together on S_2 imagine sections of the surface in fig. 2 by spheres of different radii h. (Pictures of this kind should be familiar to the fans of the Hénon-Heiles system or of the so-called rotational energy surfaces.) Going all the way to the initial phase space R_4 is easy once we remember that each point on the reduced phase space S_2 lifts to a circle in R_4. Therefore, Γ and Γ' lift to two and three equivalent regular 2-tori respectively.

3.7 Qualitative structure of quantum energy level spectrum

Quantized 2-oscillator integral n in (5) should equal $N+1$ where $1 = \frac{1}{2} + \frac{1}{2}$ is the Maslov correction for each oscillator degree of freedom and N takes integer values 0, 1, etc. Quantum number J equals $N/2$, the classical amplitude $j = \frac{1}{2}n$ satisfies quantum formula $\sqrt{J(J+1)}$ in the classical limit of $J \gg 1$ where $J(J+1) \approx (J+\frac{1}{2})^2$. The multiplet of quantum eigenstates with given N is called ***polyad*** and N is the polyad quantum number. Since our reduced phase space S_2 is compact, the number of states in each polyad is finite; for S_2^N this number equals $N+1 = 2J+1$. Quantum spectrum of the N-polyad is bracketed by the absolute maximum and minimum energy of the reduced Hamiltonian H_{red} at fixed n. These extremal energies correspond, of course, to certain stable relative equilibria (RE); in the case of the simplest Hamiltonian $\mathcal{H}$ they are $\mathcal{H}_{\Pi_{7,8}}$ and $\mathcal{H}_{\Pi_{1,2,3}}$.

Quantum wavefunctions localize near (sufficiently) stable RE. Localized wavefunctions exhibit characteristic one-dimensional nodal patterns along the corresponding periodic orbits in fig. 1, right. The number of nodes equals N. Near the energy of k equivalent RE we expect to find a quasidegenerate group of k levels split by tunneling. In the case of the simplest $D_3 \times \mathcal{T}$ invariant Hamiltonian $\mathcal{H}$ we should find doublets and triplets that form quasi-equidistant one-dimensional oscillator sequences beginning at $\mathcal{H}_{\Pi_{7,8}}$ and $\mathcal{H}_{\Pi_{1,2,3}}$ respectively. The initial spacing between the neighbors in these sequences is defined by the stabilities $\omega_{\Pi_{7,8}}$ and $\omega_{\Pi_{1,2,3}}$. The energy $\mathcal{H}_{\Pi_{4,5,6}}$ of the unstable RE separates the two sequences. Since we argued that $\omega_{\Pi_{7,8}} \gg \omega_{\Pi_{1,2,3}}$, we should expect the doublets to occupy a larger energy domain and to be more numerous and better pronounced (when J is low).

3.8 Analysis based on the normal form

We normalize (1) using the standard Lie transformation method. To order ϵ^4 (second order transformation) the normal form of (1) is[c]

$$H_{\text{n.f.}} = n - \epsilon^2\left(\frac{5}{12}n^2 - \frac{7}{3}\mu\right) - \epsilon^4\left(\frac{67}{432}n^3 + \frac{7}{36}\mu n - \frac{56}{9}\xi\right) + \dots\ , \qquad (6)$$

coefficients in the higher orders are listed below.

order	1	μn^{-2}	ξn^{-3}	$\mu^2 n^{-4}$	$\mu\xi n^{-5}$
$\epsilon^6 n^4$	$-\frac{42229}{155520}$	$-\frac{76447}{6480}$	$\frac{2093}{135}$	$\frac{115171}{1944}$	
$\epsilon^8 n^5$	$-\frac{15624833}{18662400}$	$-\frac{11656729}{2332800}$	$\frac{353843}{8100}$	$\frac{2217943}{233280}$	$\frac{6701639}{4050}$

The energies of relative equilibria are the values of this $H_{\text{n.f.}}$ at the corresponding values of (μ, ξ) in table 1,

$$H_{\Pi_{7,8}} = n + \frac{1}{6}\epsilon^2 n^2 - \frac{11}{54}\epsilon^4 n^3 + \frac{1171}{2430}\epsilon^6 n^4 - \frac{217567}{145800}\epsilon^8 n^5 \qquad (7a)$$

$$H_{\Pi_{1,2,3}} = n - \frac{5}{12}\epsilon^2 n^2 - \frac{235}{432}\epsilon^4 n^3 - \frac{38585}{31104}\epsilon^6 n^4 - \frac{2663129}{746496}\epsilon^8 n^5 \qquad (7b)$$

$$H_{\Pi_{4,5,6}} = n - \frac{5}{12}\epsilon^2 n^2 + \frac{101}{432}\epsilon^4 n^3 + \frac{108467}{155520}\epsilon^6 n^4 + \frac{35328559}{18662400}\epsilon^8 n^5 \qquad (7c)$$

Each relative equilibrium is a periodic orbit in the initial phase space R_4. It becomes an orbit of the dynamical S_1 symmetry in the transformed phase space $\tilde{R}_4$ after normalization $R_4 \to \tilde{R}_4$. The integral n is the action integral along this orbit,

$$n(h) = \frac{1}{2\pi}\oint (p_x dq_x + p_y dq_y), \qquad (8)$$

taken at fixed energy $H = h$. If we inverse the formal series (7) we obtain, therefore, the value of action (8) in the original space R_4 as a function of energy h for each nonlinear normal mode (each RE). The period of the orbits is then found as $T = 2\pi(dn/dh)$. Results are compared in fig. 3 with data obtained by numerical integration.

We can reconstruct explicitly all dynamically invariant subspaces of (the integrable approximation to) the Hénon-Heiles system. To this end we lift points on the base space S_2^J back to the total space $\tilde{R}_4$ and then use the

[c]Note, that we may differ from other authors in the choice of $\mathbf{J}$, or of its particular components. Thus Churchill and Rod obtain the same normal form (6) in terms of the components of $\mathbf{W} = 4\mathbf{J}$. They do not use $D_3 \times \mathcal{T}$–invariant polynomials μ and ξ.

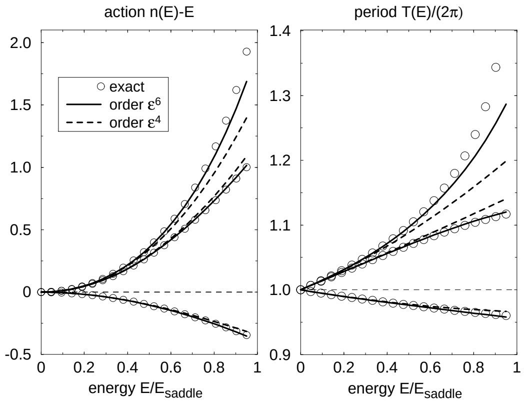

Figure 3. Action $n(E)$ and period $T(E)$ of relative equilibria (right). Solid and dashed lines show normal form approximations of order ε^6 and ε^4, circles represent exact numerical data.

formal Lie series for the inverse transformation $\tilde{R}_4 \to R_4$. From the geometric point of view, we reconstruct analytically the Hopf fibration[11] with the base S_2^J, fiber S_1, and total space S_3, which is the constant energy level set in R_4. In the simplest case of a relative equilibrium, we take just one point in S_2^J. Resulting periodic orbits in R_4 projected on the configuration plane (x, y) are shown in fig. 1. Even at high energies h they compare quite favorably to the orbits of the original non-integrable system provided that the $H_{\text{n.f.}}$ is taken to a sufficiently high order. In the general situation, we first use Euler equations of motion $\{H^J_{\text{n.f.}}(J_1, J_2, J_3), J_k\}$ in order to reconstruct the dynamics of the reduced system.

3.9 Quantized normal form

We can construct a quantum analogue of $H_{\text{n.f.}}$ in (6) if we re-express $H_{\text{n.f.}}$ as function of (J_1, J_2, J_3) using (5) and then replace (J_1, J_2, J_3) for quantum angular momentum operators. We can also return to the initial coordinates $(z, \bar{z})$ and then replace them with creation-annihilation oscillator operators[d] $(\sqrt{2}a, \sqrt{2}a^+)$. In both cases purists will accuse us of ambiguity because quantum elementary operators $(\hat{J}_1, \hat{J}_2, \hat{J}_3)$ or (a, a^+) do not commute and their correct ordering is lost in the process of normalization. Indeed, a true quantum analogue should be constructed using a parallel quantum normalization

[d] This is called the *Schwinger representation* of the angular momentum system.

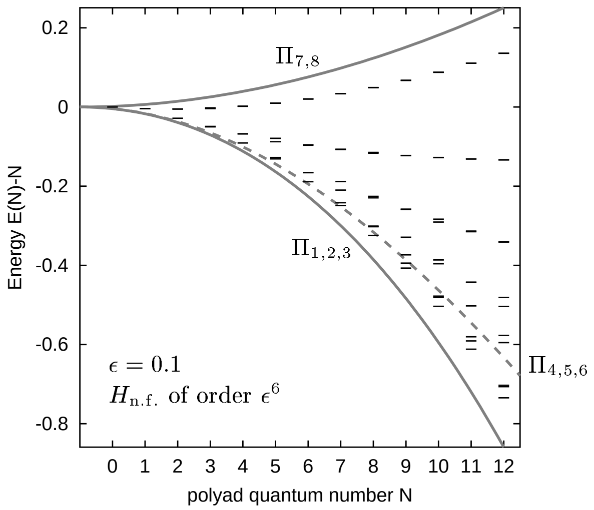

Figure 4. Energies of relative equilibria (solid and dashed lines) and quantum energy levels (bars) of the Hénon-Heiles system with $\epsilon = 0.1$ obtained using order ϵ^6 normal form $H_{\text{n.f.}}$ as functions of the polyad quantum number N, here the classical action n equals $N + 1$.

procedure known as contact or Van Vleck transformation. The general response is that our quantum $\widehat{H}_{\text{n.f.}}$ should work well in the classical limit where n is large *and* ϵ is small. In such limit, commutator corrections to the given principal order which come from higher orders of $H_{\text{n.f.}}$ can be comfortably neglected. This does not, of course, exhaust all areas of interest, but is sufficient for the illustration of our qualitative predictions.

Figure 4 shows the spectrum of $\widehat{H}_{\text{n.f.}}$ in the form of quantum-classical energy-momentum diagram. The bars which show quantum levels give positions of classical EBK 2-tori amended by tunneling. With this correction in mind, we can associate this figure with the image of the energy-momentum map in the usual sense of Cushman.[II] The larger upper part of this spectrum is occupied by doublets. The $N = 12$ polyad has three such doublets but their splitting is much too small to be reproduced in the figure. In addition, the states in the doublets realize representations $A_1 \oplus A_2$ or E of the D_3 group and in the latter case they are strictly degenerated due to symmetry. At bottom energies of large-N polyads in fig. 4 lies a triplet level. Quantum states in these triplets realize the representation $A \oplus E$, so all we can see is a doublet which is split considerably due to the low barrier energy $H_{\Pi_{4,5,6}} - H_{\Pi_{1,2,3}}$. We conclude that our qualitative predictions are indisputably correct.

4 Real atomic and molecular systems

Our atomic examples use hydrogen atom perturbed by different configurations of external electric and magnetic fields. It can be easily generalized to other perturbed Kepler systems. Our analysis of the quadratic Zeeman effect serves to establish the relation of our approach and terminology to the numerous previous work by other authors which goes back to the pioneering study of Solov'iev in 1981. Our major contribution to the study of the parallel field system is the analysis of the so-called crossover (or collapse) phenomenon[5] which can be done in the elegant style of Michel and Zhilinskií based almost entirely on the invariant theory and the orbit space analysis of simplest Hamiltonians. Our collaboration with Richard Cushman[7] on the hydrogen atom in crossed fields[6] resulted in uncovering monodromy of one of the most fundamental physical systems, in fact one of the few quantum systems where monodromy can be observed and studied experimentally.

We also consider molecular vibration and rotation-vibration systems[1,3,4]. The H_3^+ molecular ion[2] has the equilibrium configuration of an equilateral triangle. Near this equilibrium, it has three internal vibrational degrees of freedom, the "breathing" nondegenerate mode ν_1 and the doubly-degenerated "bending" mode ν_2. These modes transform according to the irreducible representations A_1 and E of the C_{3v} symmetry group of the molecule. The E-mode system at low energies is similar to the Hénon-Heiles oscillator; it has the same 8 relative equilibria. Quantum states localized near some of these modes are found in [2]. Tetrahedral molecules A_4 and AB_4 have a rich system of rotational and rotational-vibrational relative equilibria. We analyze them in detail and study the relation of the energy of relative equilibria and corresponding structure of quantum rotation-vibration energy levels to the parameters of the molecular potential.[9,10,11]

5 Concluding remarks

Our purpose was to demonstrate the influence of Louis Michel at all levels of our approach to the analysis of atomic and molecular systems. We tried to convey the taste of the intricate combination of ideas, methods, and tools, all cemented by the strong belief in the possibility and necessity to achieve an elegant and simple understanding of concrete physical problems on the basis of symmetry and topology. We shall remember Louis Michel for his great physical intuition, wide and solid mathematical background, and his courage to apply constructively the most modern mathematical theories. We hope that our work can serve as a model for further cooperation of contemporary physics and mathematics. The work continues both in the development of theory and methods and in applications to more complex systems. These new developments could only be mentioned in the talk. In particular we should pay attention to the effort of understanding quantum and classical monodromy in real systems which are only approximately integrable, and in systems with more than two degrees of freedom. We should also continue to uncover the relation between monodromy and topological quantum numbers in mixed quantum-classical systems.[8]

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