Defects of quantum state lattice and assignment of spectra

B I Zhilinskii

Université du Littoral, UMR 8101 du CNRS, 59140, Dunkerque, France

Abstract. Integer and fractional quantum monodromy is interpreted as a defect of the regular lattice of quantum states. Qualitatively different patterns of quantum states due to the presence of monodromy for integrable approximations are introduced for systems with two and three degrees of freedom. Quantum monodromy for effective Hamiltonians describing the vibrational structure of CO_2 molecule possessing 1 : 1 : 2 resonance is demonstrated as a concrete molecular example.

1. Introduction

Qualitative understanding of the dynamics of classical mechanical systems is based on the analysis of simple completely or partially integrable approximations. In a similar way, for quantum problems dealing with the discrete spectrum of finite particle systems it is important to find a system of "good" quantum numbers which can be used to label in a qualitatively correct way the eigenstates of the system. This means that we need to find a system of mutually commuting operators and to characterize eigenstates by their eigenvalues. If such approximate description is found we can represent the joint spectrum of commuting observables as a system of points in the space whose coordinate axis are values of commuting observables or equivalently, the corresponding quantum numbers. The aim or the present paper is to describe qualitatively different generic patterns present in the joint spectrum of several commuting observables using the results of the qualitative analysis of corresponding classical integrable problem.

Most qualitative characteristics of an integrable Hamiltonian dynamical system are related to the geometry of the fibration of the phase space defined by the first integrals. The Poincaré-Lyapunov-Liouville-Arnol'd theorem [1] says that for completely integrable problem the fibers are generically regular tori and the fibration is locally trivial. This means equally that locally the action-angle variables can be introduced and for the corresponding quantum problem the joint spectrum locally can be represented as a regular lattice taking into account the simplest version of the Bohr-Sommerfeld quantization rules. At the same time for many important physical systems the fibration of classical phase space induced by integrals of motion (which are mutually in involution) have singular fibers whose topology can be highly nontrivial and these singularities are stable under small deformation of system. The presence of such singularities does not allow the existence of global action-angle variables [2]. The simplest obstruction to the existence of global action-angle variables is the Hamiltonian monodromy which was analyzed in details by Duistermaat [3]. During next 20 years the Hamiltonian monodromy was studied mainly by mathematicians using several simple mathematical models like spherical pendulum [4, 5, 6]. Only recently importance of Hamiltonian monodromy became apparent to physicists and several fundamental quantum systems like hydrogen atom in external electric and magnetic fields [7], molecular ion H_2^+ [8], systems with several coupled angular momenta [9, 10] were shown to have monodromy.

From the point of view of corresponding quantum problem the absence of global action-angle variables means that the joint spectrum of commuting observables can be almost everywhere covered by local charts representing simple regular Z^N lattice with the exception of regions corresponding to the singularity of classical fibration. Such description is quite close in spirit to the description of lattices with defects [11, 12]. In what follows, we will show how to construct the defects of regular lattice which model the behavior of the joint spectrum of several commuting observables in the case of the presence of typical singularities. The first type of singularity is the so called focus-focus singularity [6, 5] which in classical mechanics is associated with presence of pinched torus as a singular fiber and has a nontrivial (integer) monodromy. Another type of singularity of classical fibration is more degenerate and consists of one parameter family of so called "curled tori" [13, 14]. This singularity is associated with fractional monodromy, whose existence was demonstrated only recently [13].

2. Quantum monodromy and defects of lattices

Let us start with regular two-dimensional (2D)-lattice L. Each vertex of the lattice L is labeled by two integers in such a way that there is an isomorphism between L and the lattice Z^2 of integer numbers. To represent the lattice we use the Cartesian coordinate system on the plane $R^2 = \{x, y\}$ and take as vertices all points with integer coordinates (n_x, n_y). We will choose as an "initial" elementary cell of the lattice the cell formed by four vertices labeled by $(n_x, n_y), (n_x+1, n_y), (n_x, n_y+1), (n_x+1, n_y+1)$. As soon as the cell is chosen we can transport the elementary cell through the lattice by making elementary steps in x or in y directions. Each elementary step consists in moving the cell by changing the n_x (or n_y) integer by one for all four vertices of the cell. Naturally for regular lattice we can transport the elementary cell with given origin (n_x, n_y) to the cell having origin at any other vertex (n'_x, n'_y). The frame is transformed in such a case by a parallel transfer over the lattice.

2.1. Integer monodromy cut

Starting from the regular Z^2 lattice in R^2 plane we suggest the following construction of the "elementary monodromy defect". Consider the set $\mathscr{C}(x:y) = \{(x,y) \in R^2 | -x > 2|y|\}$ which we call a slice. We remove the slice from the lattice and identify the points $(n_x = -2n, n_y = n) = (n_x = -2n, n_y = -n)$ for every positive integer n. We call the resulting object an "elementary monodromy defect" diagram. The origin of the removed slice is a defect point. The reason for this notation follows from the rules of the transportation of the elementary cell along a closed path surrounding the defect point and crossing once the cut [15] (see Fig. 1).

2.2. Fractional monodromy cut

We generalize this construction [15] by doing rational cut. This means that starting from some point of the lattice we do the cut with straight boundaries in such a way that we remove m

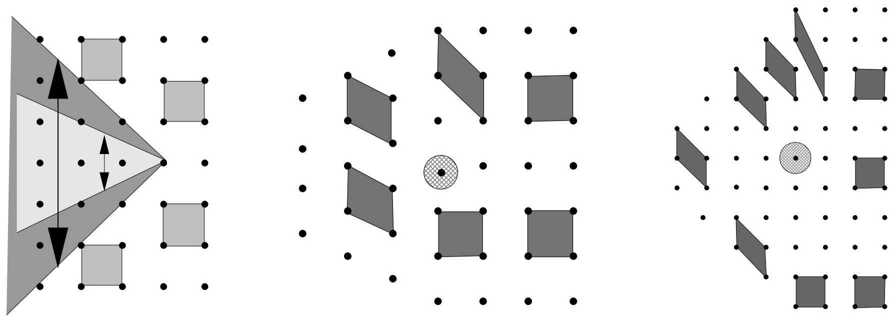

Figure 1. Construction of the monodromy defect by removing one of the slices shown on the left picture. Reconstructed lattices after removing small or large slices are shown together with transport of elementary cell along a closed path around the defect on the reconstructed lattice. The identification of boundaries after removing slice is done by the parallel shift of lattice points in vertical direction.

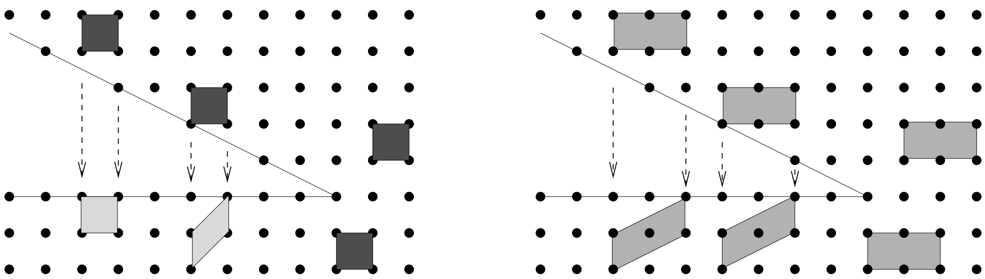

Figure 2. Construction of the $1:2$ rational lattice defect starting from the regular square lattice. (Left) - Ambiguity in the transfer of 1×1 cell through the cut. (Right) - Unambiguous transfer of double cell through the cut.

points from the n-th column. We assume that m/n is a rational number. In other words, the number of removed points from the column is assumed to be a linear function of the column number with coefficients being periodic. Such objects are known as quasi-polynomials [16]. Their application to the description of the density of quantum states via the generating function formalism is briefly reviewed in [17, 18]. Due to oscillatory contribution to the number of removed states the lattice reconstructed after such cut by parallel gliding of points till the identification of points which belong to both boundaries possesses the line rather than the point defect.

The simplest example of such construction, namely $1:2$ cut, is shown in Figure 2.

2.3. 3D-defects

Naturally, in 3D-lattices we can construct elementary codimension two defects by trivially extending to the third dimension of the 2D-defect introduced for two-dimensional section.

We restrict ourselves with an example of three elementary defects, shown schematically in Figure 3. These three defects correspond to removing following slices from the regular cubic 3D-lattice with coordinates $\{x,y,z\}$ taken along three basis vectors of the lattice:
i) The slice $|z-z_a| < n_a(y-y_a)/2$, corresponding to the negative line defect $\{z=z_a, y=y_a\}$ with amplitude n_a.
ii) The slice $|y-y_b| < n_b(x-x_b)/2$, corresponding to the negative line defect $\{y=y_b, x=x_b\}$ with amplitude n_b.

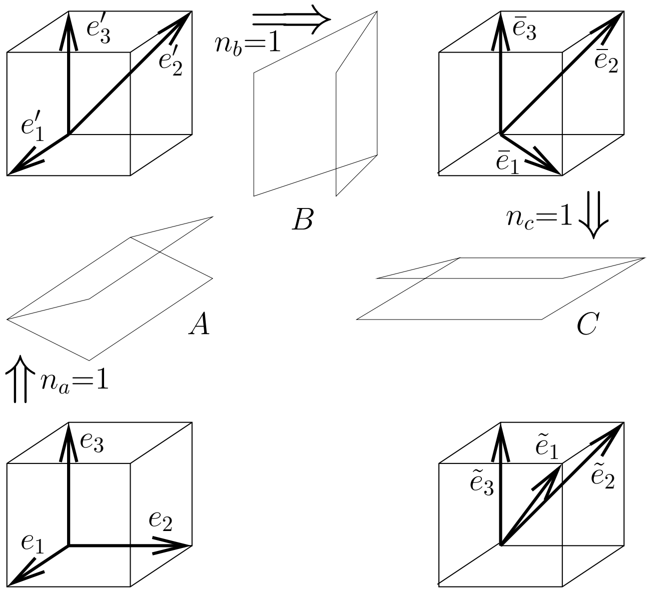

Figure 3. Transformation of 3D-cell along the closed path surrounding three elementary defects, A,B,C, represented by slices removed from the regular cubic lattice.

iii) The slice $|z-z_c| < n_c(x-x_c)/2$, corresponding to the negative line defect $\{z=z_c, x=x_c c\}$ with amplitude n_c.
We name these slices and corresponding defects simply by letters A, B, and C.

If now we take the closed path going around all three line defects and crossing cuts A,B,C in the mentioned above way (as shown in Figure 3), the resulting monodromy matrix is the product of three matrices corresponding to elementary defects and has the form

$$\begin{pmatrix} 1 & n_a & n_c \\ 0 & 1 & n_b \\ 0 & 0 & 1 \end{pmatrix}. \tag{1}$$

Figure 3 shows the transformation of the cell (more exactly of the associated frame) for the case when $n_a = n_b = n_c = 1$. Thus it is clear that with three elementary (multiple) cuts we can construct a system of defects which is globally characterized by an arbitrary unipotent $SL(3,Z)$ matrix.

3. CO_2 molecule as an example of quantum system with monodromy

The vibrational structure of CO_2 molecule gives us a non-trivial example of a physical system, which can be reasonably well described by a simplified model with mutually commuting operators exhibiting nontrivial monodromy for the joint spectrum. We remind that CO_2 molecule is a classical example of linear molecule with Fermi resonance. This means that frequency of totally symmetric stretching mode ν_1 is almost exactly equal to the double of the frequency of the degenerate bending mode ν_2. By neglecting the asymmetric stretching we get therefore the effective Hamiltonian for three degrees of freedom which is additionally invariant with respect to rotation around the molecular axis due to linearity of the equilibrium configuration

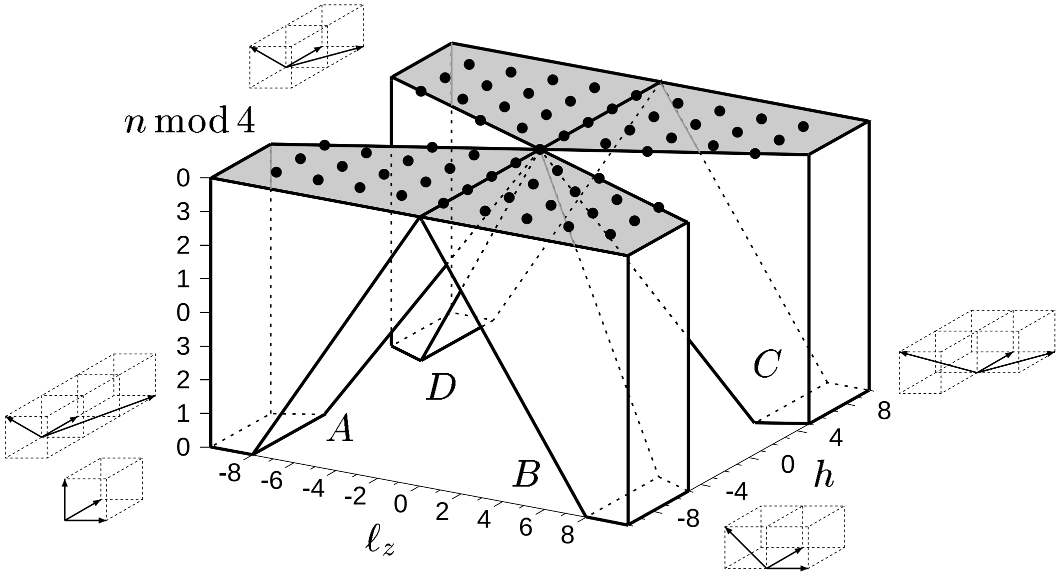

Figure 4. Regularization of the quantum state lattice for 1 : 1 : 2 resonance integrable model.

of molecule. Introducing an approximate integral of motion, the total number of vibrational quanta on all three modes, $2n_1+n_2$, which takes into account the resonance condition $\nu_1 \approx 2\nu_2$, we get the effective Hamiltonian, H, and the set of three mutually commuting observables, N, S, L, which are suitable to represent the joint spectrum.

$$H = N + \alpha S; \tag{2}$$

$$N = \tfrac{1}{2}(2p_1^2 + 2q_1^2 + p_2^2 + q^2 + p_3^2 + q_3^2), \tag{3}$$

$$S = (q_2p_3 + q_3p_2)q_1 - (q_2q_3 - p_2p_3)p_1, \tag{4}$$

$$L = \tfrac{1}{2}(p_2^2 + q_2^2 - p_3^2 - q_3^2). \tag{5}$$

Using quantum numbers n, ℓ_z, h which correspond to eigenvalues of N, L and S, the joint spectrum can be represented as forming a regular 3D-lattice with three elementary monodromy cuts and with defect for $h = l_z = 0$ [19]. The monodromy associated with closed path around this singularity follows directly from rules of transportation of an elementary cell through the cuts. The explicit form of the monodromy matrix in the basis $\{e_\ell, e_h, e_n\}$ follows directly from Figure 4. It is sufficient to compare the form of the cell in the local chart A before and after a close path surrounding the $h = \ell_z = 0$ defect: $e_\ell \to e_\ell + 2e_h;\ e_h \to e_h;\ e_n \to e_n - e_h$.

4. Conclusions

Presence of monodromy in classical Hamiltonian problems and its manifestation in corresponding quantum problem clearly demonstrate that the assignment of quantum numbers which is one of the most standard procedure in the processus of the analysis and interpretation of experimental spectroscopic and numerical *ab initio* data can be globally inapplicable. The construction of several local charts with different choices of local quantum numbers should be used in such situation. Nevertheless the question of existence or absence of global sets of quantum numbers requires detailed analysis in each concrete case because even apparently very similar problems may have completely opposite behavior. Thus, for example, the vibrational structure of LiCN molecule shows the presence of monodromy and the absence of global quantum numbers [20], whereas for HCN molecule the monodromy is absent and the global quantum numbers exist [21].

Acknowledgments

The support by the EU network MASIE, contract No. HPRN-CT-2000-00113 is acknowledged.

References

[1] Arnol'd Vl I 1989 *Mathematical Methods of Classical Mechanics* (New York: Springer-Verlag)

[2] Nekhoroshev N N 1972 *Trans. Moscow Math. Soc.* **26** 180–198

[3] Duistermaat J J 1980 *Comm. Pure Appl. Math.* **33** 687–706

[4] Cushman R H and Duistermaat J J 1988 *Bull. Am. Math. Soc.* **19** 475–479

[5] Cushman R H and Bates L M 1997 *Global aspects of classical integrable systems* (Basel: Birkhäuser)

[6] Matveev V S 1996 *Sb. Math.* **187** 495–524

[7] Cushman R H and Sadovskií D A 2000 *Physica D* **142** 166–196

[8] Waalkens H, Junge A and Dullin H R 2003 *J. Phys. A: Math. Gen.* **36** L307–L314

[9] Sadovskií D A and Zhilinskií B I 1999 *Phys. Lett. A* **256** 235–244

[10] Grondin L, Sadovskií D A and Zhilinskií B I 2002 *Phys. Rev. A* **142** 012105-1–15

[11] Mermin N D 1979 *Rev. Mod. Phys.* **51** 591–648

[12] Michel L 1980 *Rev. Mod. Phys.* **52** 617–651

[13] Nekhoroshev N N, Sadovskii D A and Zhilinskii B I 2002 *C. R. Acad. Sci. Paris, Ser. I* **335** 985–988

[14] Colin de Verdier Y and Vũ Ngọc S 2003 *Ann. Ec. Norm. Sup.* **36** 1-55

[15] Zhilinskií B I 2003 *arXiv:quant-ph*/0303181

[16] Stanley R P 1986 *Enumerative Combinatorics* (Montrey, CA: Wadsworth & Brooks/Cole) Vol. 1, Chapter 4.4

[17] Sadovski D A and Zhilinski B I 1995 *J. Chem. Phys.* **103** 10520–36

[18] Michel L and Zhilinskii B 2001 *Phys. Rep.* **341** 11–84

[19] Cushman R H, Dullin H R, Giacobbe A, Holm D D, Joyeux M, Lynch P, Sadovskii D A and Zhilinskii B I 2004 *Phys. Rev. Lett.* **93** 024302-1-4
Giacobbe A, Cushman R H, Sadovskii D A and Zhilinskii B I 2004 *J.* Math. Phys. in press

[20] Joyeux M, Sadovski D A and Tennyson J 2003 *Chem. Phys. Lett.* **382** 439–442

[21] Efstathiou K, Joyeux M and Sadovskii D A 2004 *Phys. Rev. A* **69** 032504-1–15