Reorganization of energy bands in quantum finite particle systems

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Abstract. The qualitative phenomenon of the redistribution of energy levels between bands in the energy spectrum of finite particle quantum systems (atoms and molecules) is studied from the point of view of quantum, semi-quantum and purely classical approaches. Relation with topological quantum numbers, classical and quantum monodromy, defects of regular lattices is shown.

1. Introduction

Presence of energy bands in the spectra of small atomic and molecular quantum systems is a well known characteristic feature related to existence of several typical energetic scales. Vibrational structure of electronic states, rotational structure of vibrational states, fine spin and hyperfine nuclear spin structures are simplest examples of band organization which reflect in classical terms the existence of slow and fast motions and their approximate separation. Within families of effective quantum Hamiltonians the modification of the band structure is typically observed as a result of relatively strong coupling. The purpose of the present note is to look at the phenomenon of the reorganization of energy bands under the variation of some strict or approximate integral of motion for molecular systems from several different points of view. The main idea is to understand the qualitative structure and its possible generic modifications taking into account the topological structure of the underlying classical dynamics and molecular symmetry.

Several recent review articles [1, 2, 3, 4] discuss qualitative approach to intramolecular dynamics and in particular the redistribution of energy levels between bands. We only breifly remind here the relation between redistribution, topological quantum numbers, and quantum monodromy whereas interpretation in terms of lattice defects is mainly concerned.

2. Topological quantum numbers

The relation between topological Chern numbers and the redistribution of energy levels between rotational energy bands associated with several close vibrational molecular quantum states was first conjectured in [5]. Many concrete examples of redistributions observed in real molecules were described in [6, 7], where the relation between redistribution and symmetry was emphasized, namely special symmetry selection rules for redistribution were formulated. Rigourous mathematical statement which associates to each rotational band its topological quantum number, Chern class of the complex line fibre bundle, was formulated in [8, 9]. Number of energy levels in each band was expressed in terms of the Chern class of the complex fibre bundle. This bundle characterizes the rotational structure of vibrational states in the semi-quantum model which treats rotational (slow) motion as classical and vibrational (fast) motion as quantum.

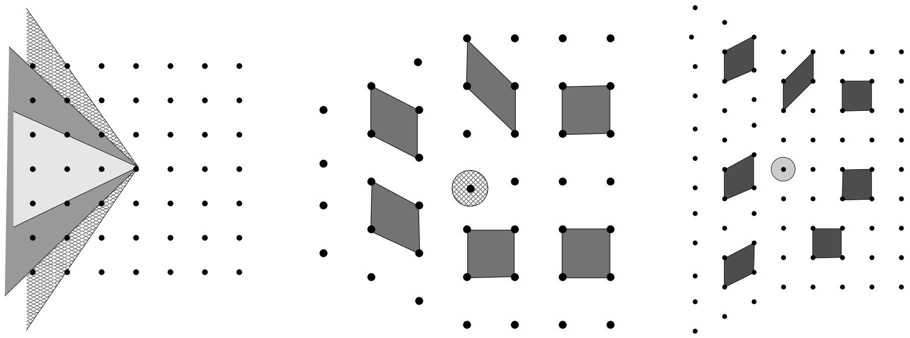

Figure 1. Construction of lattice defect by removing or adding one of the solid angles shown on the left picture. Reconnection of the lattice is done by vertical parallel shift of all vertices. The number of removed (added) vertices varies linearly. Three different angles correspond to removing (adding) respectively one, two and three vertices during the first step in the horizontal direction. On the reconstructed lattice the singularity point is shown by shadowed disk. The circular path of the elementary cell shows that removing and adding the same solid angle result in monodromy with different sign but with the same absolute value of the nondiagonal element.

Generalization of semi-quantum model to the case of effective Hamiltonians with several slow (classical) dynamical degrees of freedom leads to a new very interesting phenomenon of the formation of topologically coupled energy bands [10, 4]. Concrete model introduced in [10] deals with CP_2 (complex projective space) as the classical phase space for slow variables. The coupling with three quantum states is needed to see the formation of topologically coupled bands [4]. Number of states in the band can again be expressed through topological invariants using Atiyah-Singer index formula within, for example, Fedosov version of deformation quantization [11].

3. Quantum monodromy

Completely classical treatment [12] of the model problem of coupled angular momenta introduced in [5] to study the redistribution phenomenon shows the appearance of classical Hamiltonian monodromy [13, 14, 15] for this model problem. Manifestation of classical monodromy in corresponding quantum problem [16, 17, 12, 18] can be most easily detected if we interpret the quantum monodromy as a defect of a regular lattice of quantum states. For two degree of freedom system the evolution of elementary cell $(n_1,n_2;n_1+1,n_2;n_1+1,n_2+1;n_1,n_2+1)$ formed by quantum states with consequent quantum numbers around the singularity characterizes the monodromy and does not depend on the choice of the basis of the lattice [12, 18]. The relation between classical (quantum) monodromy and Chern indices can be seen [18] through the generalization of the Duistermaat-Heckman theorem [19]. At the same time the analogy with the description of defects in regular lattices [20, 21, 22] seems to be quite important for generalization of the quantum monodromy and corresponding phenomenon of the reorganization of energy bands.

4. Lattice defects

Lattice of quantum states with monodromy can be formally constructed in a way similar to construction of dislocations and disclinations of crystals. The presence of defect for integrable system means that global action-angle variables are not defined whereas local action-angle

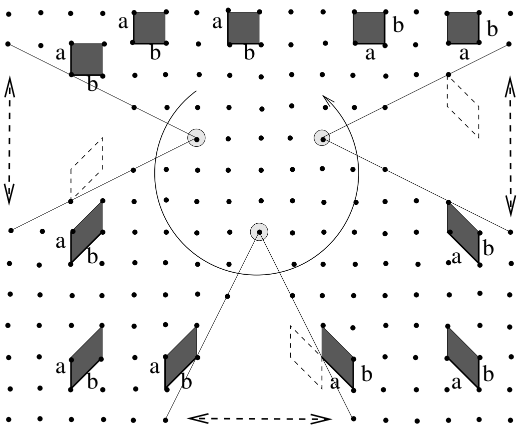

Figure 2. Regular lattice with three singular points corresponding each to elementary monodromy. For two singular points the removed solid angle is filled by vertical shift of columns of points whereas for the third singular point the shift is horizontal. The circular path around three singular points results in the rotation of the elementary cell on $\pi/2$.

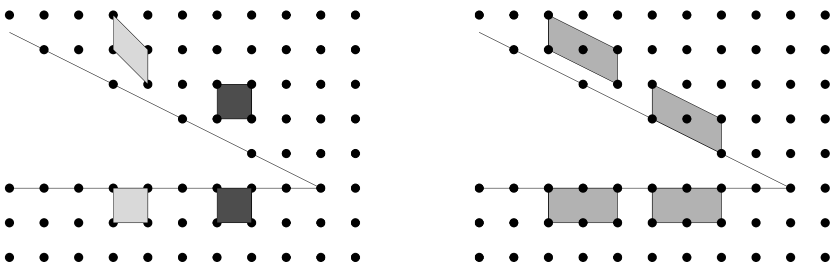

Figure 3. Reconstruction of lattice after 1:2 rational cut. The identification of two rays after cuting is done through parallel transport of vertices. Left and right figures show respectively the transfer over cut of elementary cell of dimension 1×1 and 1×2.

variables exist [23, 13]. Figure 1 illustrates the construction of lattice defect by adding or removing the same solid angle. To ensure the presence of isolated point defect for a two dimensional lattice special matching rules should be introduced to identify the two boundary of the cut. Namely, the deformation of the lattice after cut is done by parallel vertical displacement of lattice points up to identification of points on the boundary. The formation of an isolated point defect after such reconstruction is possible only for very special cuts. Three possible choices of cuts are shown in Figure 1, left. Two other subfigures show reconstructed lattices after removing and adding the smallest possible solid angle. The so obtained defects in these two cases are characterised by elementary matrices $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ or $\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$ which are defined up to conjugation with arbitrary $SL(2,Z)$ matrix due to an arbitrary choice of the lattice basis. The author of the present note has conjectured recently that only one kind of defects (associated with removing solid angle) is relevant for Hamiltonian systems. The proof of this conjecture is given in [24]. In non-Hamiltonian systems both cases of signs of elementary monodromy matrices are possible as demonstrated in [25].

It seems reasonable to conjecture further that the elementary monodromy matrix with inversed sign should appear as a generic obstruction to the existence of global quantum numbers for integrable PT-invariant non-Hermitian Hamiltonian systems [26].

In the case of multiple elementary defects the global monodromy matrix associated with the close path going around several defects can be arbitrary [27]. Figure 2 shows, for example, that three elementary $\left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right)$ defects (remind that the monodromy matrix of the defect is defined up to $SL(2,Z)$ conjugation) result in the fourth order monodromy matrix $\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$. From the point of view of crystal defects such global monodromy matrix corresponds to a $\pi/2$-disclination. In a similar way standard $\pi/3$ disclination for the triangular lattice can be constructed as a result of two defects with elementary monodromy matrices. In [27] it is proved that inversed sign monodromy matrix can be formed as a global monodromy matrix for eleven (this is in fact a minimal number of elementary defects needed for such realization) properly chosen elementary defects.

Using analogy with the "partial disclination" it is possible to form more general defects of lattice of quantum states by making a "rational cut" of the lattice. Figure 3 shows an example of such 1 : 2 cut. The reconstruction of the lattice after such cut is done again by parallel transport of vertices in vertical direction. It is important to note now that the matching rules imposed for the 1 : 2 cut result in splitting all vertices lying on the boundary of the cut in two subsets: vertices which are present on both sides of the cut and should be identified and vertices presented on one side with no partners to be identified on the another side. This leads to the line defects on the reconstructed lattice with the point defect at the top of the solid angle. The transfer of the elementary cell through the line defect can not be unambigously defined. At the same time for the 1×2 cell the monodromy is well defined but the new feature now is the appearence of half integer (rational in general) entries for the monodromy matrix [28].

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