Annals of Physics 326 (2011) 3013–3066

Contents lists available at SciVerse ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Energy bands: Chern numbers and symmetry

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ARTICLE INFO

Article history:
Received 29 June 2011
Accepted 5 July 2011
Available online 14 July 2011

Keywords:
Energy band
Fiber bundle
Chern class
Molecule

ABSTRACT

Energy bands formed by rotation–vibrational states of molecules in the presence of symmetry and their qualitative modifications under variation of some control parameters are studied within the semi-quantum model. Rotational variables are treated as classical whereas a finite set of vibrational states is considered as quantum. In the two-state approximation the system is described in terms of a fiber bundle with the base space being a two-dimensional sphere, the classical phase space for rotational variables. Generically this rank 2 complex vector bundle can be decomposed into two complex line bundles characterized by a topological invariant, the first Chern class. A general method of explicit calculation of Chern classes and of their possible modifications under variation of control parameters in the presence of symmetry is suggested. The construction of iso-Chern diagrams which split the space of control parameters into connected domains with fixed Chern numbers is suggested. A detailed analysis of the rovibrational model Hamiltonian for a D_3 invariant molecule possessing two vibrational states transforming according to the two-dimensional irreducible representation is done to illustrate non-trivial restrictions imposed by symmetry on possible values of Chern classes.

1. Introduction

Qualitative understanding of many physical phenomena is based on the construction of a model associated with topological and symmetry notions [1–3]. The interrelation between physical and mathematical ideas here is so important that many new mathematical ideas are tightly

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0003-4916/$ – see front matter
doi:10.1016/j.aop.2011.07.002

related to preliminary physical constructions [4]. The most intensive such collaboration between mathematicians and physicists is in the field of high-energy and solid state physics. The description of finite particle quantum systems (atoms and molecules) is often considered as being more related to the domain of direct extensive numerical calculation based on the study of multi-particle Schrödinger equation. Nevertheless, it turns out that many sophisticated mathematical constructions are very much adequate for the description of qualitative features of simple isolated quantum systems [5–8]. In some way the finite particle systems even have certain advantages from the point of view of the verification of the adequacy of mathematical models due to a large amount of very detailed information about energy spectra of finite quantum systems and their variation as a function of some control parameters, whereas many mathematical applications to high-energy physics, gravitation, cosmology and so on either cannot be verified experimentally at present, or can be compared with a very restrictive set of experimental data.

In this paper we discuss qualitative aspects related to such well known molecular notions as energy bands and their rearrangement from the point of view of vector bundles, their characteristic classes (Chern classes), and associated topological quantum numbers and especially from the point of view of symmetry and its consequences for the possible values of topological quantum numbers and their modifications.

The relevance of Chern numbers to the notion of reorganization of energy bands in molecules was initially suggested in [9], where the reorganization of energy bands was related to the modifications of the Chern number associated with the corresponding singularity. This initial paper was inspired by the manifestation of the "diabolic type" singularities in the adiabatic study of the evolution of quantum systems and the appearance of a geometrical Berry phase [10,11]. Further studies of essentially the same model [12–14] allowed the formulation of a more concrete relation between Chern numbers and the numbers of states in the bands. Moreover, the extension of the model to purely classical treatment reveals an interesting relation [15,16] between the redistribution of bands (accompanied by Chern number variation) and the Hamiltonian monodromy phenomenon [17–19]. This correspondence in its turn stimulated further generalizations of the Hamiltonian monodromy to the fractional monodromy phenomenon [20–22] which is ultimately related to the specific symmetry of the problem.

From the physical point of view the most spectacular appearance of the Chern numbers is related to the description of the quantum Hall effect [23,24]. Here the topological origin of Chern numbers is responsible for the appearance of a plateau of conductivity and for its persistence even in the presence of perturbations naturally existing for real materials. It was noted that the appearance of non-trivial Chern numbers for the quantum Hall effect is related to the breaking of time reversal invariance. For time reversal invariant systems new interesting topological phenomena are the quantum spin Hall effect and topological insulators [25,26]. Further attempts to classify topological phases are based on the construction of a "periodic table" taking into account the topology and symmetry of the emergent phases [27]. One of the simplest cases is the Z_2 topological invariant appearing for specific phases of topological insulators.

From the mathematical point of view the difficult part of the description of the quantum Hall effect by using Chern numbers is the description of the stratification of the set of eigenvalues and eigenfunctions of a family of Hermitian matrices [28,29,6]. Alternatively it is possible to study the singularities appearing in families of dynamical systems depending on some control parameters. In any approach the presence or absence of symmetry strongly modifies the results because the notion of a generic system itself depends on symmetry restrictions imposed on the problem. Instead of trying to develop a general equivariant formalism we study in this article several concrete examples possessing different symmetries.

We work below within the model inspired largely by molecular physics which assumes generically the existence of certain limiting cases consisting in splitting of dynamical variables (or equivalently classical motions) into several types (electronic, vibrational and rotational) which can be relatively well characterized by different scales of corresponding energy excitations, or characteristic times. In the majority of systems, due to rovibronic (rotational–vibrational–electronic) coupling the reorganization of energy levels and corresponding eigenfunctions takes place, which prevents a simple splitting of quantum energy levels and even the associated classical motions into rotational, vibrational and electronic ones [30–33].