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Band rearrangement through the 2D-Dirac equation: Comparing the APS and the chiral bag boundary conditions

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Abstract

The Dirac equation on a two-disk is studied under the chiral bag boundary condition, where the mass is treated as a parameter ranging over all real numbers. The eigenvalues as functions of the parameter are compared with those obtained under the APS boundary condition studied in a previous paper of authors (Iwai and Zhilinskii, 2015). Discrete symmetry (or pseudo-symmetry) of the boundary condition as well as the Hamiltonian is studied to explain the difference between the patterns of eigenvalues under the chiral bag and the APS boundary conditions. The spectral flow for a one-parameter family of operators is the net number of eigenvalues passing through zero in the positive direction as the parameter runs. It was demonstrated in the previous paper that the spectral flow is useful to understand the characteristic of eigenvalue pattern of the Dirac equation with the APS boundary condition. However, to capture the feature of eigenvalue pattern under the chiral bag boundary condition, one needs to introduce an extended notion of spectral flow. The eigenvalue patterns under the both boundary conditions are compared with a semi-quantum description of energy-band rearrangement.

Keywords: Energy band; Dirac equation; Chiral bag boundary condition; Spectral flow

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http://dx.doi.org/10.1016/j.indag.2015.11.010
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1. Introduction

This article is a sequel to a previous one [10]. In [10], the Dirac equation on a two-disk was treated under the APS (Atiyah–Patodi–Singer [2]) boundary condition, where the APS boundary condition requires that the boundary values of eigenstates should belong to the subspace of eigenstates associated with positive or negative eigenvalues for a chosen boundary operator. The spectral flow, which is defined for a generic one-parameter family of operators to be the net number of eigenvalues passing through zero in the positive direction as the parameter runs, is useful for the understanding of the pattern of eigenvalues as functions of the parameter. One of results of the previous article is that the spectral flow of a one-parameter family of the Dirac equation with the APS boundary condition is ± 1, depending on whether the sign of the total angular momentum eigenvalue j is positive or negative. A question arises as to whether the spectral flow is still useful for the description of the feature in the pattern of eigenvalues under another boundary condition. It will be shown that for the chiral bag boundary condition the notion of spectral flow is not applicable, since the passing through zero has no qualitative meaning for eigenvalues obtained under the chiral bag boundary condition. However, an answer to the above question will be possible if the notion of spectral flow is extended. Difference between the patterns of eigenvalues under the APS and the chiral boundary conditions can be explained by means of discrete symmetries (or pseudo-symmetries).

A further question is as to whether one can find a characteristic of band rearrangement independently of the choice of boundary conditions. This question comes from interest in the correspondence between a full quantum and a semi-quantum models. Semi-quantum models have been employed to study qualitative structure of energy bands in isolated molecules, in which the splitting of variables into two subclasses, "slow variables" and "fast variables", is assumed according to low- and high-energy excitation, and the slow and the fast variables are treated as classical and quantum ones, respectively. As long as a finite number of quantum levels are concerned, the Hamiltonian for the total system is described as a Hermitian matrix defined on a base manifold which is chosen on physical grounds. If the rotational variables are treated as classical ones, a chosen manifold is a two-sphere, which is a co-adjoint orbit of $SO(3)$ [5,11,12].

With each of disjoint eigenvalues viewed as functions on the two-sphere, is associated a complex line-bundle, which is characterized by a Chern number [5,7]. To model the band rearrangements, some control parameters are introduced into the Hamiltonian. Then, the band rearrangement is associated with a change in the Chern number accompanying the variation in the parameters. The delta-Chern was introduced in [8] to describe a change in the Chern number against the control parameters. The previous paper [10] shows that the spectral flow for the Dirac equation with the APS boundary condition naturally corresponds to the delta-Chern for a corresponding semi-quantum model. Rephrased from the viewpoint of the correspondence, a purpose of this article is to examine whether a choice of boundary condition affects the understanding of the correspondence between the full quantum and the semi-quantum models or not.

The organization of this article is as follows: Section 2 contains the setting up for solving the Dirac equation by using the method of separation of variables. Feasible solutions are given in terms of Bessel and modified Bessel functions in the radial variable as well as exponentials in the angular variable. Boundary conditions are treated in Section 3, in which the APS and the chiral bag boundary conditions are reviewed in a generic form. Section 4 includes analysis of eigenstates of the 2D-Dirac equation under the chiral bag boundary condition. Regular and edge states are found. They are described in terms of Bessel and modified Bessel functions, respectively, in the radial variable. Of particular interest are critical states, which are viewed as transient states

Please cite this article in press as: T. Iwai, B. Zhilinskii, Band rearrangement through the 2D-Dirac equation: Comparing the APS and the chiral bag boundary conditions, Indagationes Mathematicae (2015), http://dx.doi.org/10.1016/j.indag.2015.11.010