Available online at www.sciencedirect.com
SCIENCE DIRECT
PHYSICS LETTERS A
Physics Letters A 334 (2005) 363–369
www.elsevier.com/locate/pla

On the detectability of threefold degeneracies of real Hamiltonians

T. Vértesi [a,*], E. Bene [b]

[a] *Department of Theoretical Physics, University of Debrecen, Debrecen, Hungary*
[b] *Institute of Chemistry, Chemical Research Center, Hungarian Academy of Sciences, Budapest, Hungary*

Received 10 November 2004; accepted 25 November 2004

Available online 8 December 2004

Communicated by P.R. Holland

Abstract

We investigate real quantum states which are parallel-transported around a triple degeneracy. Applying a recently proposed test [Phys. Rev. Lett. 92 (2004) 060406], it is shown that when none of the states change sign upon completing the circle, the degeneracy is detectable by topological means. Examples from deformed microwave resonators are presented to illustrate the results.

PACS: 03.65.Vf; 31.50.Gh

Keywords: Geometric phases; Conical intersection; Resonators; Multiple degeneracy

1. Introduction

The work of Herzberg and Longuet-Higgins [1] implies that in order to decide whether two given potential surfaces of real Hamiltonians cross each other conically or just getting very close to each other and thereby producing an avoided crossing, one must parallel-transport the corresponding adiabatic eigenvectors along a closed path round the point in question. If and only if both of the eigenvectors change sign then the point must be twofold degenerate formed by a conical intersection.

The question we intend to pose is the following: Can we construct a robust method as well when three states intersect, i.e., can the above method, suitable for the crossing of two states be generalized for threefold degeneracies? The purpose of the present Letter is to investigate this possibility and thereby to give an answer for the question above.

It can be yet shown in the spin-j system in the presence of an adiabatically rotating magnetic field [3], that the generalization for dimension $n > 2$ is not straightforward, and needs more considerations. In this case when the field sweeps out the solid angle 2π,

* Corresponding author.
E-mail address: tvertesi@heavy-ion.atomki.hu (T. Vértesi).

0375-9601/$ – see front matter
doi:10.1016/j.physleta.2004.11.046

we obtain common sign changes for all eigenvectors. The sign is equal to $+1$ or -1 depending on the parity of $n = 2j + 1$. Especially for spin-1 (when $n = 3$) none of the eigenvectors change sign, that is the sign change pattern is $(+1, +1, +1)$, where ± 1 at the ith position means that the wave function corresponding to the ith lowest eigenvalue did (-1) or did not $(+1)$ change sign after the cyclic adiabatic evolution. The above spin-1 result implies that the threefold degeneracy pertaining to this pattern is not detectable by the mean of inspecting the sign changes. On the other hand Lauber et al. [4] performed experiments on a microwave cavity, involving a triple degeneracy in its rectangular geometry. By deforming its shape adiabatically around the point corresponding to the undeformed geometry in the two-dimensional space of deformations, this experiment has yielded the pattern $(-1, +1, -1)$. This means that only the sideward wave functions change sign and indicates that this particular threefold degeneracy is detectable by the usual topological means. Although we remark that indeed the particular experiment of Lauber et al., as it was pointed out in Ref. [6], involved two additional 'satellite' degeneracies in the looping circle, but the cyclic phases of the pattern are not affected by them.

As we saw that either the pattern $(+1, +1, +1)$ or the pattern $(-1, +1, -1)$ can be observed in real physical systems which possess triple degeneracy, we can raise the question whether any other sign combinations can occur in addition to them. Recently, Manolopoulos and Child [5] answered this problem based upon investigating the model Hamiltonian which scales linearly in the vicinity of a general n-fold degeneracy, and concluded that the set of permitted sign change patterns for $n = 3$ are exactly the above-cited $(+1, +1, +1)$ and $(-1, +1, -1)$ ones, and no other sign-change combinations are allowed.

In order to generalize the observability of twofold conical degeneracies to n-fold $(n > 2)$ ones, it is sufficient to be concerned with degeneracies, where the corresponding pattern contains common $+1$ elements. This follows from the fact, that the presence of degeneracy can be revealed by inspection of the sign-change pattern, whenever at least one eigenstate changes sign after a full revolution. Thus specifically for a triple degeneracy we further need to study the system pertaining to the pattern $(+1, +1, +1)$. Since in this case the emerging real Berry phases [3] do not carry useful information about the presence of degeneracy, we wonder if any more information can be inferred from the behavior of wave functions on the loop encircling the point of degeneracy. Recently, Johansson and Sjöqvist [9] examined just this possibility, and put forward a topological test, which can be also applied to this special case, furthermore they also proved that this test is optimal in exploiting all topological information concerning the existence of degeneracies inside the loop. Now our aim is to apply this topological test, which can be considered as the generalization of Longuet-Higgins' sign change theorem [2] to the case of pattern $(+1, +1, +1)$ and we intend to show that the theorem of Ref. [9] will manage to signal the presence of triple degeneracy.

The Letter is organized as follows. In the next section we recall the theorem of Ref. [9] specializing the general method to the case which fits to our context. We investigate small contours encircling threefold intersections, mapping to loops in $SO(3)$. We apply some results from Ref. [5] and walk on the strand of Ref. [9] to determine the homotopy classes of the corresponding loops. In Section 3 the theoretical findings are illustrated with numerical calculations for microwave resonators, based on the examples of Ref. [5]. Then in Section 4 we generalize the previous results to contours encircling finite area round the degeneracy, and finally we conclude the present work in Section 5.

2. Classification of nontrivial loops in $SO(3)$ with the test of Johansson and Sjöqvist

Let us suppose a 3-fold degeneracy at the origin of the two-dimensional (x, y) parameter space of a system with real Hamiltonian. Writing the Hamiltonian of the system in a fixed $|\{i\}\rangle_{i=1}^{3}$ basis of the three-dimensional Hilbert space, it can be represented by a 3×3 parameter dependent symmetric matrix. The Taylor expansion of the Hamiltonian $H(x, y)$ about the origin of the parameter space is given by [7]

$$H(x, y) = fx + gy + O\big(x^2, y^2\big), \tag{1}$$

here $f = \frac{\partial H}{\partial x}(0, 0)$ and $g = \frac{\partial H}{\partial y}(0, 0)$. In a sufficiently small neighborhood of the origin the first-order approximation applies, hence we can write $F = fr$ and