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Duals of Crystallographic Groups. Band and Quasi-Band Representations

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Abstract. Band representations are analyzed from a pure group theoretical point of view, with the aid of the dual of the crystallographic group (the set of equivalence classes of unitary irreducible representations). It is shown on the examples of the one-dimensional crystallographic groups that we have to introduce a distinction between band and quasi-band representations, the word *band* being reserved for induced representations.

The dual of the group F222 is explicitly constructed. It permits to show that two elementary band representations which have the same decompositions into unitary irreducible representations are not equivalent.

1. Introduction

Generally, in physics, the crystallographic groups (also called space groups) are studied not as abstract groups but from their Euclidean properties, that is from crystals. However, many of their properties can be investigated from a strictly group theoretical point of view. Here, we propose to present some interesting facts concerning the orthorhombic face centered group F222 (number 22 in the International Tables for Crystallography [1]). The main parts of the work which is presented here are i) the construction of the dual, that is the space of all classes of irreducible representations of the group and ii) the analysis of some band representations [2–12]. In many respects, such an approach is different from the one based on the Brillouin zone and Hamiltonian theory. From the point of view of representation theory, the Brillouin zone is an object which provides a nice way of constructing the unitary irreducible representations of the space group but, although it is related with the open part of the dual, it hides all properties of band representations which are essentially related with the topological structure of the dual. Another inconvenience of the Brillouin

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