6. WREATH PRODUCTS AND THE SYMMETRY OF INCOMMENSURATE CRYSTALS

Daniel B. Litvin

Department of Physics
The Pennsylvania State University
The Berks Campus
Reading, PA 19608, USA

Introduction

In the context of magnetic and non-magnetic crystallographic space groups, the symmetry of a three-dimensional incommensurate crystal is not a three-dimensional group, but a group of lower dimensionality. The symmetry group of the non-magnetic crystal 1T-$TaSe_2$, with its incommensurate structural distortion[1], is a one-dimensional space group. The symmetry group of the magnetic crystal $MnAu_2$, with its incommensurate spiral spin-arrangement[2], and the symmetry group of α - $TbAu_2$, with its incommensurate linear transverse-wave spin arrangement[3], are two-dimensional groups.

We introduce a new class of crystallographic groups, named "wreath groups," based on the concept of wreath products of groups. We show that the symmetry group of a three-dimensional incommensurate crystal is a three-dimensional wreath group.

Wreath Products of Groups[4,5]

Let $\mathcal{P}$ be a group, H a set, and $\tilde{G}$ a group homomorphic onto a subgroup $\theta_{\tilde{G}}$ of the group of all permutations of H. Let $\mathcal{P}^H = \mathcal{P}x\mathcal{P}x..x\mathcal{P}$ taken H times. Elements of $\mathcal{P}^H$ are functions f on H whose values are in $\mathcal{P}$. $\tilde{G}$ is homomorphic onto a group $\Phi_{\tilde{G}}$ of automorphisms of $\mathcal{P}^H$ where $\phi_G f(h) = f(\theta_G^{-1}h)$.

The wreath product of the groups $\mathcal{P}$ and $\tilde{G}$ is denoted by $\mathcal{P} \textcircled{w} \tilde{G}$ and is the semi-direct product $\mathcal{P}^H \textcircled{s}_{\phi} \tilde{G}$. Elements of this group are denoted by $(f \,||\, G)$, and the product of two elements is given by:

$$(f \,||\, G)(f' \,||\, G') = (f \cdot \phi_G f' \,||\, GG')$$

where $f \cdot \phi_G f'(h) = f(h) \cdot f'(\theta_G^{-1}h)$.

Wreath Groups

Let $\vec{S}(r)$ be a static spin arrangement defined on a crystal $C_s(3)$. Let H be the subset $C_s(3)$ of the three-dimensional euclidean space $E_s(3)$, i.e. the subset consisting of all atomic positions r, $\tilde{G}$ the space group of the crystal, and $\tilde{P}$ the vector space $\tilde{V}_1^+$, considered as a group under vector addition. We denote f(h) by $\vec{V}(r)$. Elements of the wreath product are then denoted by $(\vec{V}(r) \parallel G)$, and the product of two elements is written, using an additive notation for the product of functions $\vec{V}(r)$, as:

$$(\vec{V}(r) \parallel G)(\vec{V}'(r) \parallel G') = (\vec{V}(r) + \vec{V}'(G^{-1}r) \parallel GG')$$

An element $(\vec{V}(r) \parallel G)$ of the wreath product is defined to transform a spin arrangement $\vec{S}(r)$ into the spin arrangement denoted by $(\vec{V}(r') \parallel G)\vec{S}(r)$ and defined by:

$$(\vec{V}(r') \parallel G)\vec{S}(r) = \vec{S}(G^{-1}r) + \vec{V}(r)$$

The subgroup of all elements of the wreath product such that

$$(\vec{V}(r') \parallel G)\vec{S}(r) = \vec{S}(r)$$

is called the "wreath group" of the spin arrangement.

The wreath group of a spin arrangement defined on a crystal $C_s(3)$ of space group symmetry $\tilde{G}$ is isomorphic to $\tilde{G}$. The elements of the wreath group are denoted by $(\vec{V}_G(r) \parallel G)$ where:

$$\vec{V}_G(r) = \vec{S}(r) - \vec{S}(G^{-1}r)$$

Consequently, the symmetry group of an incommensurate spin arrangement defined on a three-dimensional crystal is a three-dimensional wreath group.

Example: α-$TbAu_2$

The wreath group of the spin arrangement in α-$TbAu_2$ is a three-dimensional wreath group of elements $(\vec{V}_G(r) \,||\, G)$. G is an element of the space group $\tilde{G}$ = I4/mmm (D_{4h}^{17}). The functions $\vec{V}_G(r)$ are defined by the above equation with

$$\vec{S}(r) = \hat{z}S\cos(\vec{Q}\cdot\vec{r} + \beta)$$

where $\vec{Q} = Q(\hat{x} + \hat{y})/\sqrt{2}$, the wavelength $\lambda = 2\pi/Q$ being incommensurate with the crystalline lattice, and β is a phase factor.

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