

Neutron Scattering in Condensed Matter Physics II

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Series 3 - Representation analysis of Magnetic Structures

For the centrosymmetric and orthorhombic space group $Pbnm$ (D_{2h}^{16}) one finds eight different one-dimensional representations for a magnetic structure associated with the wave vector $\mathbf{k} = 0$.

	e	2_x	2_y	2_z	$\bar{1}$	$2_x\bar{1}$	$2_y\bar{1}$	$2_z\bar{1}$
$\Gamma_1 = \Gamma_{1g}$	1	1	1	1	1	1	1	1
$\Gamma_2 = \Gamma_{2g}$	1	1	-1	-1	1	1	-1	-1
$\Gamma_3 = \Gamma_{3g}$	1	-1	1	-1	1	-1	1	-1
$\Gamma_4 = \Gamma_{4g}$	1	-1	-1	1	1	-1	-1	1
$\Gamma_5 = \Gamma_{1u}$	1	1	1	1	-1	-1	-1	-1
$\Gamma_6 = \Gamma_{2u}$	1	1	-1	-1	-1	-1	1	1
$\Gamma_7 = \Gamma_{3u}$	1	-1	1	-1	-1	1	-1	1
$\Gamma_8 = \Gamma_{4u}$	1	-1	-1	1	-1	1	1	-1

Assume four spins S_j ($j = 1 - 4$) at the four equivalent centres of symmetry $(0\ 0\ 0)$, $(0\ 0\ 1/2)$, $(1/2\ 1/2\ 1/2)$ and $(1/2\ 1/2\ 0)$. The $3 \cdot 4 = 12$ dimensional vector space can be decomposed using the irreducible representations Γ_j ($j = 1 - 4$):

$$\Gamma^{12D} = 3\Gamma_1 + 3\Gamma_2 + 3\Gamma_3 + 3\Gamma_4.$$

Applying a projection operation along the x direction one obtains the following basis functions:

$$A_x = S_{1x} - S_{2x} - S_{3x} + S_{4x}$$

$$F_x = S_{1x} + S_{2x} + S_{3x} + S_{4x}$$

$$C_x = S_{1x} + S_{2x} - S_{3x} - S_{4x}$$

$$G_x = S_{1x} - S_{2x} + S_{3x} - S_{4x}$$

Find for each basis function the corresponding irreducible representation. Proceed as shown in the example during the lecture.