PUA representations of Shubnikov space groups and selection rules

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I. Introduction

The aim of this paper is to study selection rules for processes in crystalline solids where an external uniform magnetic field is present. When there is no field these selection rules are well known ([1], [2]). In the presence of an external uniform magnetic field we have to consider projective representations of the symmetry group of the system instead of vectorrepresentations ([3], [4]). Since we will also consider time-reversal symmetry our symmetry group will be a Shubnikov space group of type I or III. We suppose that the finite-dimensional projective unitary-antiunitary (PUA) representations of the Shubnikov space groups of types I and III are known [5], and that they are derived with the method of generalised induction given by Shaw and Lever [6]. In section II we give some properties of induced PUA representations, analogous to well-known ([1], [2]) properties of induced vectorrepresentations. The selection rules are then derived in section III.

II. Properties of induced PUA representations

Let G be a finite group, G_o a subgroup of G of index 1 or 2, and H a subgroup of G. A PUA representation of G is a mapping D from G into the unitary matrices which satisfies $D(g)\,D(g')^g = \sigma(g,g')\,D(gg')$ for some mapping σ: $G \times G \to U(1)$ where $D^g = D$ if $g \in G_o$ and $D^g = D^*$ if $g \notin G_o$, the asterisk denoting complex conjugation. The mapping σ is called the factor system of D. Two PUA representations D and D' of G with the same factor system are equivalent if there exists a unitary matrix U with the property $D'(g) = U^{-1}D(g)U^g$ for all $g \in G$. In the sequel we shall identify equivalent PUA representations. If Δ is a PUA representation of H with factor system σ, then Δ_g, defined by $\Delta_g(ghg^{-1}) = \sigma(ghg^{-1},g)\,\sigma^*(g,h)\,\Delta^g(h)$ is a PUA representation of $H_g \equiv gHg^{-1}$ with factor system σ. The PUA representation of G which is induced from the PUA representation Δ of H, both with factor system σ, will be denoted by $\Delta \uparrow_\sigma G$. Let K also be a subgroup of G. Then we can write $G = \sum_i K g_i H$ where $\{g_i\}$ is a fixed set of doublecoset representatives containing the identity e of G. In the sequel we give without proof some properties of induced PUA representations. The following notation will be used: ω and σ are factor systems of G; Γ and Λ are PUA representations of G and K respectively with factor system ω, and Δ is a PUA representation of H with factor system σ.

Theorem I: If σ is the trivial factor system of G then $\Delta \uparrow_\sigma G$ does not contain the trivial UA representation of G if and only if Δ does not contain the trivial UA representation of H.

Theorem II: $\Gamma \otimes (\Gamma \uparrow_\sigma G) = [(\Gamma \downarrow H) \otimes \Delta] \uparrow_{\omega\sigma} G$

Theorem III: If $H \subseteq K \subseteq G$ then $(\Delta \uparrow_\sigma K) \uparrow_\sigma G = \Delta \uparrow_\sigma G$

Theorem IV: $(\Delta \uparrow_\sigma G) \downarrow K = \sum_i [(\Delta_{g_i} \downarrow (H_{g_i} \cap K)) \uparrow_\sigma K]$

<u>Theorem V</u>: $(\Delta \uparrow_{\sigma} G) \times (\Lambda \uparrow_{\omega} G) = \sum_{i} \{ [(\Delta_{g_i} \downarrow (H_{g_i} \cap K)) \otimes (\Lambda \downarrow (H_{g_i} \cap K))] \uparrow_{\omega\sigma} G \}$

We conclude this section with a theorem which is nothing but a repeated application of theorem V, but which is of great importance in the next section.

<u>Theorem VI</u>: Let M be another subgroup of G; ν another factor system of G and Ξ an irreducible PUA representation of M with factor system ν. For each g_i we can write $G = \sum_j (H_{g_i} \cap K) g_{j,i} M$. Let $N_{j,i}$ be the subgroup $M_{g_{j,i}} \cap H_{g_i} \cap K$. Then

$$(\Xi \uparrow_{\nu} M) \otimes (\Delta \uparrow_{\sigma} G) \times (\Lambda \uparrow_{\omega} G) = \sum_i \sum_j \{ [(\Xi_{g_{j,i}} \downarrow N_{j,i}) \otimes (\Delta_{g_i} \downarrow N_{j,i}) \otimes (\Lambda \downarrow N_{j,i})] \uparrow G \}$$

III. Selection rules for an electron in a crystal with a uniform magnetic field

We consider an electron in a crystalline solid where an external uniform magnetic field is present. The symmetry group G of the system is a Shubnikov space group of type I or III. H is the subgroup of translations of G and G_o the nonmagnetic subgroup of G. Elements of G will be denoted by $(\vec{t},R)$ where $\vec{t} \in H$ and $R \in K \equiv G/H$. We define $(\vec{t},R)$ by its action on space-time: $(\vec{t},R)(\vec{x};t) = (R\vec{x} + \vec{t} + \vec{t}_R, \varepsilon_R t)$ where ε_R is defined by $\varepsilon_R = 1$ if $R \in K_o \equiv G_o/H$ and $\varepsilon_R = -1$ if $R \notin K_o$ and $\vec{t}_R$ is a fixed non-primitive translation associated with R. The multiplication of elements of G is now given by $(\vec{t},R)(\vec{t}',R') = (\vec{t} + R\vec{t}' + \vec{m}(R,R'), RR')$ where the mapping $\vec{m}$: $K \times K \to H$ is given by $\vec{m}(R,R') = \vec{t}_R + R\vec{t}_{R'} - \vec{t}_{RR'}$. Let $\vec{t}_1, \vec{t}_2$ and $\vec{t}_3$ be basic translations of H. Then each element $\vec{t}$ of H can be written as $\vec{t} = n_1\vec{t}_1 + n_2\vec{t}_2 + n_3\vec{t}_3$. In the sequel we shall identify $\vec{t}$ with the columnvector with entries n_1, n_2 and n_3. Moreover each element R of K is given by the 3x3-matrix which represents R with respect to the basic vectors.

Since G is an infinite group and it is convenient to work with finite groups we apply periodic boundary conditions. This is, however, only possible when the magnetic field $\vec{B}$ is in the direction of some translation $\vec{t}$ of H and satisfies $\vec{B} = \frac{2\pi\hbar c}{e\Omega} a\vec{t}$ where Ω is the volume of a primitive cell and a is a rational number [3]. From now on we suppose that $\vec{B}$ has this properties and assume tacitly that periodic boundary conditions are applied, which enables us to consider G as a finite group. Moreover we choose the basic translations such that $\vec{t}_3$ is in the direction of $\vec{B}$. The Hilbert space $\mathcal{H}$ of wavefunctions $\psi(\vec{x},t)$ satisfying the Schrödinger equation $H\psi = i\hbar\frac{\partial}{\partial t}\psi$ where $H = \frac{1}{2m}(\vec{p} - \frac{e}{c}\vec{A}(\vec{x}))^2 + e\Phi(\vec{x})$ carries a PUA representation of G with factor system σ. The equivalence class of σ is determined by the magnetic field and is independent of the choice of the gauge of the potentials. We may choose σ from its equivalence class in such a way that [7]

$$\sigma((\vec{t},R),(\vec{t}',R')) = \gamma(\vec{t},R\vec{t}')\ \gamma(\vec{t}+R\vec{t}', \vec{m}(R,R'))\ \nu(R,R')\ \ P(R,\vec{t}')$$

where γ, the restriction of σ to $H \times H$ is given by [3]

$$\gamma(\vec{t},\vec{t}') = \exp\{-2\pi i\ \frac{m}{2N}\ (t_1t_2' - t_2t_1')\}$$

Here we wrote $\frac{m}{N}$ for the rational number a, and we suppose that m and N have no common factor.

We are interested in matrix elements $(\phi_j^{\nu}, O_k^{\mu}\ \phi_{\ell}^{\rho})$. Here the functions $\{\phi_i^{\gamma}, i=1,\ldots, \dim D^{\gamma}\}$ form a basis for the irreducible PUA representation D^{γ} of G with factor system σ and O^{μ} is an irreducible tensor operator transforming according

to the irreducible UA representation D^μ of G. The matrix element $(\phi_j^\nu, O_k^\mu \phi_\ell^\rho)$ is equal to zero due to the symmetry of the system if the trivial UA representation of G does not occur in the triple direct product $D^\mu \otimes D^{\nu *} \otimes D^\rho$.
Suppose D^μ, D^ν and D^ρ are equal to $\Delta^\mu {\uparrow_1} G$, $\Delta^\nu {\uparrow_\sigma} G$ and $\Delta^\rho {\uparrow_\sigma} G$ respectively, where Δ^μ, Δ^ν and Δ^ρ are allowable PUA representations of the little groups M, H and K of the irreducible PU representations $\mathcal{D}^\mu$, $\mathcal{D}^\nu$ and $\mathcal{D}^\rho$ of H respectively. $\mathcal{D}^\mu$ is given by $\mathcal{D}^\mu(\vec{t}) = \exp(2\pi i \vec{k}''.\vec{t})$ and $\mathcal{D}^\nu$ and $\mathcal{D}^\rho$ are N-dimensional and given by vectors $\vec{k}'$ and $\vec{k}$ respectively (equation 4.9 of [5]). We may assume that the allowable PUA representation Δ has the form $\Delta(\vec{t},R) = \mathcal{D}(\vec{t})U(R) \otimes E(R)$ [5]. Let $G = \sum_i K(\vec{e},R_i)H$; $H_i = (\vec{e},R_i)H(\vec{e},R_i)^{-1}$; $G = \sum_j (H_i \cap K)(\vec{e},R_{j,i})M$; $M_{j,i} = (\vec{e},R_{j,i})M(\vec{e},R_{j,i})^{-1}$; $N_{j,i} = G_o \cap M \cap H_i \cap K$; $\Delta_i^\nu = \Delta^\nu_{(\vec{e},R_i)}$ and $\Delta_{j,i}^\mu = \Delta^\mu_{(\vec{e},R_{j,i})}$. Then, using theorems I and VI, it follows that $D^\mu \otimes D^{\nu *} \otimes D^\rho$ does not contain the trivial UA representation of G iff the trivial representation of $N_{j,i}$ is not contained in $\Delta_{j,i}^\mu \otimes \Delta_i^{\nu *} \otimes \Delta^\rho$ for each value of i and j; thus, iff $\sum_{N_{j,i}} \mathrm{Tr}\, \Delta_{j,i}^\mu(\vec{t},R)\, \mathrm{Tr}\, \Delta_i^{\nu *}(\vec{t},R)\, \mathrm{Tr}\, \Delta^\rho(\vec{t},R) = 0 \ \forall i,j$. Let H_1 be the subgroup of H consisting of the elements $\vec{t}$ with t_1 and t_2 multiples of N. We write $\vec{t} = \vec{s} + \vec{w}$ for each $\vec{t} \in H$, with $\vec{s} \in H_1$ and $0 \leq w_{1,2} < N$ and $w_3 = 0$. Then $(\vec{t},R) = (\vec{s},E)(\vec{w},R)$. In the sum above we will carry out the summation over $\vec{s}$. After some calculations, using the equations (3.2)-(3.6) of [7] and equation (3.16) of [8], and writing $\vec{s} = Q\vec{t}_o$ where Q is the diagonal 3x3-matrix with $Q_{11} = Q_{22} = N$ and $Q_{33} = 1$ we find that the sum contains a term $\sum_{\vec{t}_o} \exp\{2\pi i\, \vec{t}_o.[\vec{k} - \epsilon_{R_i} Q R_i^{-1T} Q^{-1} \vec{k}' + \epsilon_{R_{j,i}} Q R_{j,i}^{-1T} \vec{k}'' - Q\vec{k}(R_i) + \epsilon_{R_i} \vec{p}(R_i)]\}$
Here the vectors $\vec{k}(R_i)$ are parameters of the factorsystem σ and are determined by the magnetic field (equation (3.16) of [8]; Note that the matrices B^{R_i}, also occurring in this equation are zero due to the fact that the magnetic field is not changed under the operations of group G). The vectors $\vec{p}(R_i)$ are given by $p_j(R_i) = \frac{m}{2N}(R_i^{-1})_{1j}(R_i^{-1})_{2j} Q_{jj}^2$.
Due to the periodic boundary conditions we finally obtain the selection rule that $\vec{k} - \epsilon_{R_i} Q R_i^{-1T} Q^{-1} \vec{k}' + \epsilon_{R_{j,i}} Q R_{j,i}^{-1T} \vec{k}'' - Q\vec{k}(R_i) + \epsilon_{R_i} \vec{p}(R_i) = 0 \pmod 1$ for some i and j is a necessary condition in order to have non-zero matrix elements.

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