Summary. The transformation properties of irreducible tensor operators and the applicability of the Wigner-Eckart theorem to finite magnetic groups have been studied.

1 Introduction

Selection rules and ratio of intensities for transitions between different states of a physical system are obtained from the appropriate matrix elements of operators between the initial and the final states of the system [1, 2]. The calculation of the matrix elements becomes simplified if one invokes the Wigner-Eckart theorem [3, 4, 5]. This theorem introduces the concept of a set of operators that transforms according to some irreducible representation of the appropriate symmetry group of the system. For compact and for finite groups, if the Kronecker inner direct
product of two irreducible representations contains any irreducible representation only once, the matrix element of such an operator between states belonging to irreducible representations will be proportional to the corresponding Clebsch-Gordan (CG) coefficient, the proportionality constant being called the reduced matrix element. The proof of this theorem depends on the fact that the matrix element when transformed by a symmetry element of the system has the same value as the untransformed matrix element. If the symmetry group of the system is a magnetic group, then antilinear elements are present and for these elements the transformed matrix elements are complex conjugate of the untransformed value. For this reason the Wigner-Eckart theorem is not in general valid in the case of magnetic groups. Recently Backhouse [6] and Doni and Paravicini [7] have investigated the theory of selection rules in magnetic crystals whose symmetry group contains antilinear elements. We have here investigated the conditions when the Wigner-Eckart theorem is valid for symmetry groups containing antilinear elements. To this end we have studied the transformation laws of irreducible tensor operators (both linear and antilinear) for magnetic groups. In order that the results can be applied to spinor cases as well, projective corepresentations [8, 9] have been considered. Previously Aviran and Zak [10] have investigated this problem. Their results are somewhat complicated because a quadratic relationship between the CG coefficients was used in their analysis, whereas a linear relationship has been used here.

2 Irreducible tensor operators

Here we give transformation laws of irreducible tensor operators for a magnetic group [8, 9]

\[
M(G) = G \cup a_0 G, \quad a_0^2 \in G,
\]

where \( a_0 \) is an antilinear element and \( G \) is a group of linear elements. The corepresentation \( D^\lambda(\alpha) \), \( \alpha \in M(G) \), belonging to the cofactor system \( \lambda(\alpha, \beta) \), \( \alpha, \beta \in M(G) \) satisfies [8, 9]

\[
\begin{align*}
D^\lambda(\alpha) D^\lambda(\beta) [\alpha] & = \lambda(\alpha, \beta) [\alpha\beta] D^\lambda(\alpha\beta), \\
\lambda(\alpha, \beta) [\gamma] \lambda(\alpha\beta, \gamma) & = \lambda(\alpha, \beta\gamma) \lambda(\beta, \gamma), \\
|\lambda(\alpha, \beta)| & = 1.
\end{align*}
\]

We have used the square bracket symbol \([\alpha]\) everywhere, so that

\[
A[\alpha] = \begin{cases} 
A, & \text{if } \alpha \text{ is linear,} \\
A^*, & \text{if } \alpha \text{ is antilinear,}
\end{cases}
\]
where $A$ is a matrix, an operator, or a complex number.

We define the Wigner operator $O_\alpha$, $\alpha \in M(G)$, by the relation

$$O_\alpha O_\beta = \lambda(\alpha, \beta)^{[\alpha\beta]} O_{\alpha\beta}. \tag{3}$$

This relation is satisfied when $O_\alpha$s operate on the bases belonging to the appropriate cofactor system. For proper rotations characterized by the Eulerian angles ($\alpha, \beta, \gamma$)

$$O_{(\alpha, \beta, \gamma)} = \exp(-i\alpha J_z) \exp(-i\beta J_y) \exp(-i\gamma J_z), \tag{4}$$

where $J_i$s are the usual angular momentum operators. The relation (3) will be automatically satisfied if we take the appropriate bases belonging to the vector corepresentation or the spinor corepresentation. For the time reversal operator $\theta$, which is antilinear, its action on the spin states $|j, m\rangle$ will be given by

$$O_\theta |j, m\rangle = (-1)^j-m |j, -m\rangle. \tag{5}$$

The $m$-th component of any tensor operator belonging to the $\mu$-th irreducible corepresentation of the cofactor system $\lambda(\alpha, \beta)$, which may be either linear or antilinear, will transform as

$$T_{\lambda\mu}^m (\alpha) = \lambda\left(\alpha^{-1}, \alpha\right)^{[T]} O_\alpha T_{\lambda\mu}^m O_{\alpha^{-1}} = \sum_n D_{nm}^{\lambda\mu} (\alpha)^{[T]} T_{n\mu}. \tag{6}$$

This relation will also cover the case when $T$ is antilinear. For the sake of completeness we write here the transformation relation of the bases belonging to the $\mu$-th irreducible corepresentation of the same factor system $\lambda(\alpha, \beta)$

$$|\Phi_{\lambda\mu}^m (\alpha)\rangle = O_\alpha |\Phi_{m\mu}^\lambda \rangle = \sum_n D_{nm}^{\lambda\mu} (\alpha) |\Phi_{n\mu}^\lambda \rangle. \tag{6a}$$

Thus

$$T_{\lambda\mu}^m (\alpha) |\Phi (\alpha)\rangle = O_\alpha T_{\lambda\mu}^m |\Phi \rangle. \tag{6b}$$

The result of successive action of two operators $O_\beta$ and $O_\alpha$ will be given by

$$O_\alpha O_\beta T_{\lambda\mu}^m O_{\beta^{-1}}^{[\beta]} O_{\alpha^{-1}}^{[\alpha]} = \lambda(\alpha, \beta)^{[\alpha\beta]} \frac{\lambda(\alpha^{-1}, \alpha) \lambda(\beta^{-1}, \beta)^{[\alpha]}}{\lambda(\beta^{-1}\alpha^{-1}, \alpha\beta)} \cdot O_{\alpha\beta} T_{\lambda\mu}^m O_{\beta^{-1}\alpha^{-1}}^{[\alpha\beta]} \tag{7}$$

The proof is a straightforward application of Eq. (2) for the choice $\lambda(\alpha, e) = \lambda(e, \alpha) = 1$.

The irreducible tensors $T_{\lambda\mu}^m$ can be obtained by the operation of the projection operator $P_{\lambda\mu}^m$ on an arbitrary tensor $T$

$$T_{\lambda\mu}^m = P_{\lambda\mu}^m T = \sum_{\alpha \in M} D_{\alpha m\alpha}^{\lambda\mu} (\alpha)^{[T]} \lambda\left(\alpha^{-1}, \alpha\right)^{[T]} O_\alpha T O_{\alpha^{-1}}^{[\alpha]}, \tag{8}$$
where \( m_0 \) is any fixed index.

Incidentally, the projection operator \( P^\lambda_\mu_m \), which operating on an arbitrary state \( |\Phi\rangle \) will give the \( m \)-th basis of the \( \mu \)-th irreducible corepresentation belonging to the cofactor system \( \lambda (\alpha, \beta) \) has the same form \[^{[16]}\] as for the vector corepresentation.

\[
P^\lambda_\mu_m = \sum_{\alpha \in M} D^\lambda_\mu_{m\alpha} (\alpha^\ast) O_\alpha.
\]

(9)

\section{Wigner-Eckart theorem}

For groups with linear elements the Wigner-Eckart theorem \[^{[3]}\] states that under the restriction given in Sec. \[^{[1]}\]

\[
\langle \Phi^\lambda_\mu_{m_1} | T^\lambda_\mu_{m_2} | \Phi^\lambda_\mu_{m_3} \rangle = \frac{1}{d^\lambda_\mu_{m_3}} \langle \lambda_1 \mu_1 \| | \lambda_2 \mu_2 \| \lambda_3 \mu_3 \rangle \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 \| \lambda_3 \mu_3 m_3 \rangle ,
\]

(10)

where \( \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 \| \lambda_3 \mu_3 m_3 \rangle \) is the CG coefficient defined by the relation

\[
\langle \Phi^\lambda_\mu_{m_1} \rangle = \sum_{m_1 m_2} \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 \| \lambda_3 \mu_3 m_3 \rangle \langle \Phi^\lambda_\mu_{m_1} \rangle |\Phi^\lambda_\mu_{m_2} \rangle .
\]

(11)

The reduced matrix element is defined by

\[
\langle \lambda_1 \mu_1 \| | \lambda_2 \mu_2 \| \lambda_3 \mu_3 \rangle = \sum_{n_1 n_2 n_3} \langle \lambda_1 \mu_1 n_1; \lambda_2 \mu_2 n_2 \| \lambda_3 \mu_3 n_3 \rangle^\ast \langle \Phi^\lambda_\mu_{n_1} | T^\lambda_\mu_{n_2} | \Phi^\lambda_\mu_{n_3} \rangle
\]

(12)

and \( d^\lambda_\mu_{m_3} = \) the dimension of the irreducible corepresentation \( D^\lambda_\mu_{m_3} \).

The CG coefficient is zero unless \( \lambda_3 (\alpha, \beta) = \lambda_1 (\alpha, \beta) \lambda_2 (\alpha, \beta) \).

For magnetic groups no such simple relation is, in general, true. We now investigate the conditions for the validity of such a theorem for magnetic groups. We note that

\[
\langle \Phi^\lambda_\mu_{m_1} (\alpha) | T^\lambda_\mu_{m_2} (\alpha) | \Phi^\lambda_\mu_{m_3} (\alpha) \rangle = \sum_{n_1 n_2 n_3} \langle \Phi^\lambda_\mu_{n_1} | T^\lambda_\mu_{n_2} | \Phi^\lambda_\mu_{n_3} \rangle \times
\]

\[
D^\lambda_\mu_{m_1} (\alpha)^\ast D^\lambda_\mu_{m_2} (\alpha)^{[T]} D^\lambda_\mu_{m_3} (\alpha)^{[T]} .
\]

(13)

Case 1. \( T \) is a linear operator.

In this case the matrix element on the left-hand side of Eq. \[^{[13]}\] is zero unless

\[
\lambda_3 (\alpha, \beta) = \lambda_1 (\alpha, \beta) \lambda_2 (\alpha, \beta) , \quad \forall \alpha, \beta \in M (G).
\]

(14)
Using the transformation relation (6) and (6a) for $T^\lambda_m (\alpha)$ and $\Phi^\lambda_m (\alpha)$ and the linear equations (Eq. (27) of Ref. [11]) satisfied by the CG coefficients of a magnetic group

$$
\sum_{m_1 m_2} \left[ \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3 \rangle \sum_{u \in G} D^\lambda_{i_1 m_1} (u) D^\mu_{i_2 m_2} (u) D^\nu_{i_3 m_3} (u) \right] \\
+ \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3' \rangle \sum_{a \in M - G} D^\lambda_{i_1 m_1} (a) D^\mu_{i_2 m_2} (a) D^\nu_{i_3 m_3} (a) \\
= \frac{|M|}{d_{\lambda \mu \nu}} \delta_{m_3, m_3'} \langle \lambda_1 \mu_1 i_1; \lambda_2 \mu_2 i_2 | \lambda_3 \mu_3 i_3 \rangle, \quad (15)
$$

we get

$$
\sum_{m_1 m_2} \left[ \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3' \rangle \sum_{u \in G} \langle \Phi^\lambda_{m_1} (u) T^\mu_{m_2} (u) | \Phi^\nu_{m_3} (u) \rangle \\
+ \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3 \rangle \sum_{a \in M - G} \langle \Phi^\lambda_{m_1} (a) T^\mu_{m_2} (a) | \Phi^\nu_{m_3} (a) \rangle \\
= \frac{|M|}{d_{\lambda \mu \nu}} \delta_{m_3, m_3'} \sum_{n_1 n_2 n_3} \langle \lambda_1 \mu_1 n_1; \lambda_2 \mu_2 n_2 | \lambda_3 \mu_3 n_3 \rangle \langle \Phi^\lambda_{n_1} T^\mu_{n_2} | \Phi^\nu_{n_3} \rangle, \quad (16)
$$

where $|M|$ = the order of the magnetic group $M (G)$.

In expressing

$$
\langle \Phi^\lambda_{m_1} (\alpha) T^\mu_{m_2} (\alpha) | \Phi^\nu_{m_3} (\alpha) \rangle
$$

in Eq. (16) we shall use the identity [11]

$$
\langle O_{\alpha_1} z_1 \Phi_1 | O_{\alpha_2} z_2 \Phi_2 \rangle = z_1^{* \alpha_1} z_2^{\alpha_2} \langle \Phi_1 | O_{\alpha_1^{-1} \alpha_2} \Phi \rangle \langle \alpha_1, \alpha_2 \rangle
$$

with

$$
\langle \Phi_1 | O_{\alpha_1^{-1} \alpha_2} \Phi \rangle \langle \alpha_1, \alpha_2 \rangle = \begin{cases} \\
\langle \Phi_2 | O_{\alpha_2^{-1} \alpha_1} \Phi_1 \rangle & \text{if both } \alpha_1, \alpha_2 \in M - G \\
\langle \Phi_1 | O_{\alpha_1^{-1} \alpha_2} \Phi_2 \rangle & \text{otherwise}
\end{cases}
$$

(17)

where $\Phi_i$s are state vectors and $z_i$s are complex numbers. We observe that the expression on the left-hand side of Eq. (16) is real and we can write

$$
\frac{1}{2} \sum_{m_1 m_2} \left[ \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3 \rangle \langle \Phi^\lambda_{m_1} T^\mu_{m_2} | \Phi^\nu_{m_3} \rangle \\
+ \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3 \rangle \langle \Phi^\lambda_{m_1} T^\mu_{m_2} | \Phi^\nu_{m_3} \rangle \right] \\
= \frac{1}{d_{\lambda \mu \nu}} \delta_{m_3, m_3'} \langle \lambda_1 \mu_1 | \lambda_2 \mu_2 | \lambda_3 \mu_3 \rangle_L, \quad (17a)
$$
where for a linear operator $T$ the reduced matrix element is given by

$$\langle \lambda_1 \mu_1 || \lambda_2 \mu_2 || \lambda_3 \mu_3 \rangle_L = \sum_{n_1 n_2 n_3} \langle \lambda_1 \mu_1 n_1; \lambda_2 \mu_2 n_2 | \lambda_3 \mu_3 n_3 \rangle^* \langle \Phi^{\lambda_1 \mu_1}_{n_1} \mid T^{\lambda_2 \mu_2}_{n_2} \mid \Phi^{\lambda_3 \mu_3}_{n_3} \rangle. \quad (18)$$

These will be the equations satisfied by the matrix elements. The CG coefficients satisfy the orthogonality relations $[11]$

$$\sum_{m_1 m_2 m_1' m_2'} \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3 \rangle^* \langle \lambda_1 \mu_1 m_1'; \lambda_2 \mu_2 m_2' | \lambda_3 \mu_3 m_3' \rangle^* \times$$

$$\langle \lambda_1 \mu_1 m_1' | \lambda_1 \mu_1 m_1 \rangle \langle \lambda_2 \mu_2 m_2' | \lambda_2 \mu_2 m_2 \rangle = \delta_{\mu_3 \mu_3'} \langle \lambda_3 \mu_3 m_3' | \lambda_3 \mu_3 m_3 \rangle \quad (19)$$

It should be noted that the bases belonging to either a type (a) or a type (c) corepresentation $[3]$ are all orthogonal $[11]$. Thus if none of the 3 corepresentations $\mu_1, \mu_2 : \mu_3$ are of Wigner type (b), then

$$\langle \Phi^{\lambda_1 \mu_1}_{m_1} \mid T^{\lambda_2 \mu_2}_{m_2} \mid \Phi^{\lambda_3 \mu_3}_{m_3} \rangle = \frac{1}{d_{\lambda_3 \mu_3}} \langle \lambda_1 \mu_1 || \lambda_2 \mu_2 || \lambda_3 \mu_3 \rangle_L \langle \lambda_1 \mu_1 m_1; \lambda_2 \mu_2 m_2 | \lambda_3 \mu_3 m_3 \rangle, \quad (20)$$

is a solution of Eq. (18). If any of the 3 corepresentations appearing in the matrix element is of type (b), then the corresponding matrix element is a linear combination of terms proportional to the CG coefficients. Even when they are valid, Eq. (20) will be unique only if the CG coefficients obtained from Eq. (15) are unique $[11]-[14]$. The CG coefficients are unique if and only if

$$\det |L (i_1 i_2 i_3, m_1 m_2 m_3) + A (i_1 i_2 i_3, m_1 m_2 m_3) - \delta_{i_1 m_1} \delta_{i_2 m_2} \delta_{i_3 m_3}| = 0$$

and

$$\det |L (i_1 i_2 i_3, m_1 m_2 m_3) - A (i_1 i_2 i_3, m_1 m_2 m_3) - \delta_{i_1 m_1} \delta_{i_2 m_2} \delta_{i_3 m_3}| = 0$$

where

$$L (i_1 i_2 i_3, m_1 m_2 m_3) = \frac{d_{\lambda \mu \nu}}{|M|} \sum_{u \in G} D_{i_1 m_1}^{\lambda_1 \mu_1} (u) D_{i_2 m_2}^{\lambda_2 \mu_2} (u) D_{i_3 m_3}^{\lambda_3 \mu_3} (u)^*$$

and

$$A (i_1 i_2 i_3, m_1 m_2 m_3) = \frac{d_{\lambda \mu \nu}}{|M|} \sum_{a \in M - G} D_{i_1 m_1}^{\lambda_1 \mu_1} (a) D_{i_2 m_2}^{\lambda_2 \mu_2} (a) D_{i_3 m_3}^{\lambda_3 \mu_3} (a)^*. \quad(21)$$

In the case of groups having no antilinear operators if we replace the second summand on the left-hand side of Eq. (17a) by the first summand we get the set of linear equations satisfied by the matrix elements. Since in these cases the bases are all orthogonal and the CG coefficients are essentially unique Eq. (20) is an exact relation $[15]-[16]$. 

6
In the previous analysis we have assumed that in the expansion of the Qroneker inner direct product of two irreducible corepresentations \( D^{λ_1μ_1} \) and \( D^{λ_2μ_2} \) the irreducible corepresentation \( D^{λ_3μ_3} \) occurs only once. When there are more than one repetition, the different repetitions of \( D^{λ_3μ_3} \) in the decomposition of the inner product representation are characterized by \( \langle λ_1μ_1 i_1; λ_2μ_2 i_2 | τ_3λ_3μ_3 i_3 \rangle \). As has been shown in [11] the CG coefficients for different \( τ_3 \)'s satisfy equations similar to Eq. (15). So similar considerations will be valid for \( \langle \Phi_{i_3}^{λ_1μ_1} | T_{i_2}^{λ_2μ_2} | Ψ_{i_3}^{λ_3μ_3} \rangle \).

But in general the most we can tell about a quantum mechanical state \( | Ψ_{i_3}^{λ_3μ_3} \rangle \) is that it transforms as the \( i - 3 \)-th component of the irreducible corepresentation \( D^{λ_3μ_3} \). In this case

\[
| Ψ_{i_3}^{λ_3μ_3} \rangle = \sum_{τ_3} a_{τ_3} | Φ_{i_3}^{τ_3λ_3μ_3} \rangle
\]

and

\[
\langle \Phi_{i_3}^{λ_1μ_1} | T_{i_2}^{λ_2μ_2} | Ψ_{i_3}^{λ_3μ_3} \rangle = \sum_{τ_3} a_{τ_3} \langle \Phi_{i_3}^{λ_1μ_1} | T_{i_2}^{λ_2μ_2} | Φ_{i_3}^{τ_3λ_3μ_3} \rangle.
\]

The quantum mechanical matrix element for the transition probability is thus a linear combination of terms each of which is a product of a reduced matrix element \( \langle λ_1μ_1 || λ_2μ_2 || τ_3λ_3μ_3 \rangle \) and the corresponding CG coefficient \( \langle λ_1μ_1 i_1; λ_2μ_2 | τ_3λ_3μ_3 i_3 \rangle \).

**Case 2.** \( T \) is an antilinear operator.

In this case the matrix element on the left-hand side of Eq. (13) is zero unless

\[
λ_2 (α, β) = λ_1 (α, β) λ_3 (α, β).
\]

An analysis similar to that for Case 1 will show that the matrix elements will satisfy the relations

\[
\frac{1}{2} \sum_{m_1 m_3} \left[ \langle λ_1μ_1 m_1; λ_3μ_3 m_3 | λ_2μ_2 m_2' \rangle \langle Φ_{m_1}^{λ_1μ_1} | T_{m_2}^{λ_2μ_2} | Φ_{m_3}^{λ_3μ_3} \rangle^* \right] + \langle λ_1μ_1 m_1; λ_3μ_3 m_3 | λ_2μ_2 m_2 \rangle \langle Φ_{m_1}^{λ_1μ_1} | T_{m_2}^{λ_2μ_2} | Φ_{m_3}^{λ_3μ_3} \rangle
\]

\[
= \frac{1}{d_{λ_2μ_2}} δ_{m_2, m_2} \langle λ_1μ_1 || λ_2μ_2 || λ_3μ_3 \rangle_{AL},
\]

where the reduced matrix element for an antilinear operator \( T \) is

\[
\langle λ_1μ_1 || λ_2μ_2 || λ_3μ_3 \rangle_{AL} = \sum_{n_1 n_2 n_3} \langle λ_1μ_1 n_1; λ_3μ_3 n_3 | λ_2μ_2 n_2 \rangle \langle Φ_{n_1}^{λ_1μ_1} | T_{n_2}^{λ_2μ_2} | Φ_{n_3}^{λ_3μ_3} \rangle.
\]

When none of these corepresentations are of type (b) according to Wigner’s classification [3], then

\[
\langle Φ_{m_1}^{λ_1μ_1} | T_{m_2}^{λ_2μ_2} | Φ_{m_3}^{λ_3μ_3} \rangle = \frac{1}{d_{λ_2μ_2}} \langle λ_1μ_1 || λ_2μ_2 || λ_3μ_3 \rangle_{AL} \langle λ_1μ_1 m_1; λ_3μ_3 m_3 | λ_2μ_2 m_2 \rangle.
\]
is a solution. The condition for essential uniqueness of this factorization is given by a relation similar to Eq. (21) if the indices 2 and 3 there are interchanged. For linear groups again, the relation (24) is exact.

In case of repetition of $D^{\lambda_2 \mu_2}$ in the decomposition of the inner direct product representation $D^{\lambda_1 \mu_1} \otimes D^{\lambda_3 \mu_3}$ the same considerations as in the case of linear $T$ will hold.

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P. M. van den Broek has kindly pointed out that even for corepresentations of type (b), the bases are orthogonal; hence the results obtained here are true for all the three types of corepresentations.