PHY 745 Group Theory
11-11:50 AM MWF Olin 102

Plan for Lecture 28:

Time reversal symmetry and
Magnetic groups
Chap. 16 in DDJ

1. **Effects of time reversal symmetry on point groups and space groups**
2. **Effects of magnetic configurations on point groups and space groups**

Note: These slides contain materials from an electronic version of the Dresselhaus textbook.

	Fri: 03/17/2017		*APS Meeting - no class*		
23	Mon: 03/20/2017	Chap. 7.7	Jahn-Teller Effect	#15	03/24/2017
24	Wed: 03/22/2017	Chap. 7.7	Jahn-Teller Effect		
25	Fri: 03/24/2017		Spin 1/2	#16	03/27/2017
26	Mon: 03/27/2017		Dirac equation for H-like atoms	#17	03/29/2017
27	Wed: 03/29/2017	Chap. 14	Angular momenta	#18	03/31/2017
28	Fri: 03/31/2017	Chap. 16	Time reversal symmetry	#19	04/07/2017
29	Mon: 04/03/2017				
30	Wed: 04/05/2017				
31	Fri: 04/07/2017				
32	Mon: 04/10/2017				
33	Wed: 04/12/2017				
	Fri: 04/14/2017		*Good Friday Holiday -- no class*		
34	Mon: 04/17/2017				
35	Wed: 04/19/2017				
36	Fri: 04/21/2017				
	Mon: 04/24/2017		Presentations I		
	Wed: 04/26/2017		Presentations II		

Time reversal symmetry in physics:

$-t \leftrightarrow t$

There are many examples of physical systems in which the behavior at time t and at time $-t$ are the same. For example, in absence of a magnetic field or of internal spin, the time dependent Schoedinger equation:

$$H\psi = i\hbar\frac{\partial \psi}{\partial t} \quad \leftrightarrow \quad H\psi^* = i\hbar\frac{\partial \psi^*}{\partial(-t)}$$

Denote time reversal operator as $\hat{T}$

$$\hat{T}\psi(\vec{r},t) = \psi(\vec{r},-t) = \psi^*(\vec{r},t).$$

Properties of the time-reversal symmetry

The important properties of the time reversal operator include:

1. commutation: $[\hat{T}, \mathcal{H}] = 0$
   Because of **energy conservation**, the time reversal operator $\hat{T}$ commutes with the Hamiltonian $\hat{T}\mathcal{H} = \mathcal{H}\hat{T}$. Since $\hat{T}$ commutes with the Hamiltonian, eigenstates of the time reversal operator are also eigenstates of the Hamiltonian.

2. anti-linear: $\hat{T}i = -i\hat{T}$
   From Schrödinger's equation (Eq. 21.1), it is seen that the reversal of time corresponds to a change of $i \to -i$, which implies that $\hat{T}i = -i\hat{T}$. We call an operator **anti-linear** if its operation on a complex number yields the complex conjugate of the number rather than the number itself $\hat{T}a = a^*\hat{T}$.

3. action on wave functions: $\hat{T}\psi = \psi^*\hat{T}$
   Since $\hat{T}\psi = \psi^*\hat{T}$, the action of $\hat{T}$ on a scalar product is

$$\hat{T}(\psi, \phi) = \int \phi^*(\vec{r})\psi(\vec{r})d^3r\ \hat{T} = (\psi, \phi)^*\hat{T} \qquad (21.4)$$

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More details

For a wavefunction not involving electron spin

$\hat{T} = \hat{K}$ (complex conjugation)

For a wavefunction including spin:

$$\hat{T} = \hat{K}\sigma_y \qquad \text{where } \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Commutation relations with time reversal:

Coordinates: $T\mathbf{r} = \mathbf{r}T$

Momenta: $T\mathbf{p} = -\mathbf{p}T$

Spin: $T\boldsymbol{\sigma} = -\boldsymbol{\sigma}T$

Krammer's theorem: All energy levels of a system containing an odd number of electrons must be at least doubly degenerate (unless magnetic fields remove the degeneracy.

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Effects of time reversal symmetry on point groups

Consider a point group with h members $\{R_i\}$ with basis functions ψ_α :

For representation $D^i_{\alpha\beta}(R_k)$: $\psi_\alpha = \sum_\beta D^i_{\alpha\beta}(R_k)\psi_\beta$

What about $D^i_{\alpha\beta}(TR_k)$?

Wigner's possibilities:

a. ***D*** and ***D**** are equivalent to the same real irreducible representation.
b. ***D*** and ***D**** are inequivalent.
c. ***D*** and ***D**** are equivalent but cannot be made real.

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Wigner's possibilities:

a. ***D*** and ***D**** are equivalent to the same real irreducible representation.
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c. ***D*** and ***D**** are equivalent but cannot be made real.

Example:

Table 21.1: Character table for point group C_4.

C_4 (4)			E	C_2	C_4	C_4^3	Time reversal
x^2+y^2, z^2	R_z, z	A	1	1	1	1	(a)
x^2-y^2, xy		B	1	1	-1	-1	(a)
(xz, yz)	(x,y)	E	1	-1	i	$-i$	(b)
	(R_x, R_y)		1	-1	$-i$	i	(b)

Some details:

We can distinguish three different possibilities in the case of **no spin**:

(a) All of the matrices in the representation D can be written as real matrices. In this case, the time reversal operator leaves the representation D invariant and no additional degeneracies in $E(\vec{k})$ result.

(b) If the representations D and D^* cannot be brought into equivalence by a unitary transformation, there is a doubling of the degeneracy of such levels due to time reversal symmetry. Then the representations D and D^* are said to form a **time reversal symmetry pair** and these levels will stick together.

(c) If the representations D and D^* can be made equivalent under a suitable unitary transformation, but the matrices in this representation cannot be made real, then the time reversal symmetry also requires a doubling of the degeneracy of D and the bands will stick together.

Time reversal symmetry effects on the group of the wavevector

Suppose $Q_0\mathbf{k} = -\mathbf{k}$

$Q_0^2\mathbf{k} = \mathbf{k}$

Note that if inversion is a member of the group, then Q_0 corresponds to inversion. Otherwise Q_0 may not be a member of the group of the wavevector.

Possibilities according to C. Herring:

$$\begin{aligned}\textstyle\sum_{Q_0} \chi(Q_0^2) &= h \quad \text{case (a)} \\ &= 0 \quad \text{case (b)} \\ &= -h \quad \text{case (c)}\end{aligned}$$

Effects of time reversal symmetry on a Bloch state

$$\hat{T}\psi_{n,k\uparrow}(\vec{r}) = \psi_{n,-k\downarrow}(\vec{r})$$

so that the time reversal conjugate states are

$$E_{n\uparrow}(\vec{k}) = E_{n\downarrow}(-\vec{k})$$

and

$$E_{n\downarrow}(\vec{k}) = E_{n\uparrow}(-\vec{k}).$$

If inversion symmetry exists as well,

$$E_n(\vec{k}) = E_n(-\vec{k})$$

then

$$E_{n\uparrow}(\vec{k}) = E_{n\uparrow}(-\vec{k}) \text{ and } E_{n\downarrow}(\vec{k}) = E_{n\downarrow}(-\vec{k})$$

Table 21.2: Summary of rules regarding degeneracies and time reversal.

Case	Relation between D and D^*	Frobenius-Schur test	Spinless electron	Half-integral spin electron
Case (a)	D and D^* are equivalent to the same real irreducible representation	$\sum_R \chi(Q_0^2) = h$	No extra degeneracy	Doubled degeneracy
Case (b)	D and D^* are inequivalent	$\sum_R \chi(Q_0^2) = 0$	Doubled degeneracy	Doubled degeneracy
Case (c)	D and D^* are equivalent to each other but not to a real representation	$\sum \chi(Q_0^2) = -h$	Double degeneracy	No extra degeneracy

Examples:

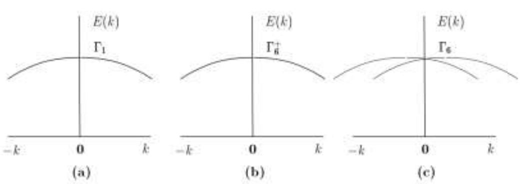

Figure 21.2: Schematic example of Kramers degeneracy in a crystal in the case of: (a) no spin-orbit interaction where each level is doubly degenerate (↑, ↓), (b) both spin-orbit interaction and inversion symmetry are present and the levels are doubly degenerate, (c) spin-orbit interaction and no spatial inversion symmetry where the relations 21.23 and 21.24 apply.

Examples:

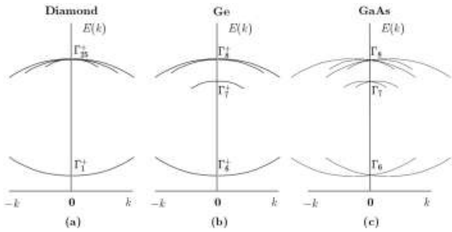

Figure 21.3: Schematic examples of energy bands $E(\vec{k})$ in diamond, Ge and GaAs near $\vec{k} = 0$. (a) Without spin-orbit coupling, each band in diamond has a two-fold spin degeneracy. (b) Splitting by spin-orbit coupling in Ge, with each band remaining doubly degenerate. (c) Splitting of the valence bands by the spin-orbit coupling in GaAs. The magnitudes of the splittings are not to scale.

Table 21.3: Character table for C_4

C_4	E	$\bar{E}$	C_4	$\bar{C}_4$	C_2	$\bar{C}_2$	C_4^{-1}	$\bar{C}_4^{-1}$	Time Inv.	Bases for C_4
Γ_1	1	1	1	1	1	1	1	1	a	z or S_z
Γ_2	1	1	-1	-1	1	1	-1	-1	a	xy
Γ_3	1	1	i	i	-1	-1	$-i$	$-i$	b	$-i(x+iy)$ or $-(S_x+iS_y)$
Γ_4	1	1	$-i$	$-i$	-1	-1	i	i	b	$i(x-iy)$ or (S_x-iS_y)
Γ_5	1	-1	ω	$-\omega$	i	$-i$	$-\omega^3$	ω^3	b	$\phi(1/2,1/2)$
Γ_6	1	-1	$-\omega^3$	ω^3	$-i$	i	ω	$-\omega$	b	$\phi(1/2,-1/2)$
Γ_7	1	-1	$-\omega$	ω	i	$-i$	ω^3	$-\omega^3$	b	$\phi(3/2,-3/2)$
Γ_8	1	-1	ω^3	$-\omega^3$	$-i$	i	$-\omega$	ω	b	$\phi(3/2,3/2)$

$$i = e^{i\pi/2} \qquad \omega = e^{i\pi/4}$$

Some details

	E	$\bar{E}$	C_4	$\bar{C}_4$	C_2	$\bar{C}_2$	C_4^{-1}	$\bar{C}_4^{-1}$
Γ_5:	ω^0	ω^4	ω	ω^5	ω^2	ω^6	ω^7	ω^3
Γ_6:	ω^0	ω^4	ω^7	ω^3	ω^6	ω^2	ω	ω^5
Γ_7	ω^0	ω^4	ω^5	ω	ω^2	ω^6	ω^3	ω^7
Γ_8:	ω^0	ω^4	ω^3	ω^7	ω^6	ω^2	ω^5	ω

Application of the Frobenius–Schur test for Γ_5 yields:

$$\begin{aligned}\sum \chi(Q_0^2) &= (1)(-1) + (1)(-1) - \omega^2 - \omega^2 + 1 + 1 - \omega^6 - \omega^6 \\ &= -1 - 1 - i - i + 1 + 1 + i + i = 0\end{aligned}$$

Table 21.4: Character Table and Basis Functions for the Group D_{3d}

	D_{3d}	E	$\bar{E}$	$2C_3$	$2\bar{C}_3$	$3C_2'$	$3\bar{C}_2'$	I	$\bar{I}$	$2S_6$	$2\bar{S}_6$	$3\sigma_d$	$3\bar{\sigma}_d$	Time Inv.	Bases
L_1^+	Γ_1^+	1	1	1	1	1	1	1	1	1	1	1	1	a	R
L_2^+	Γ_2^+	1	1	1	1	−1	−1	1	1	1	1	−1	−1	a	S_z
L_3^+	Γ_3^+	2	2	−1	−1	0	0	2	2	−1	−1	0	0	a	$(S_x - iS_y)$, $-(S_x + iS_y)$
L_1^-	Γ_1^-	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	a	zS_z
L_2^-	Γ_2^-	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	a	z
L_3^-	Γ_3^-	2	2	−1	−1	0	0	−2	−2	1	1	0	0	a	$(x - iy)$, $-(x + iy)$
L_6^+	Γ_4^+	2	−2	1	−1	0	0	2	−2	1	−1	0	0	c	$\phi(1/2,-1/2)$
L_4^+	Γ_5^+	1	−1	−1	1	i	$-i$	1	−1	−1	1	i	$-i$	b	$\phi(3/2,-3/2)$ $-i\phi(3/2,3/2)$
L_5^+	Γ_6^+	1	−1	−1	1	$-i$	i	1	−1	−1	1	$-i$	i	b	$-(\phi(3/2,3/2)$ $-i\phi(3/2,-3/2))$
L_6^-	Γ_4^-	2	−2	1	−1	0	0	−2	2	−1	1	0	0	c	$\Gamma_4^+ \times \Gamma_1^-$
L_4^-	Γ_5^-	1	−1	−1	1	i	$-i$	−1	1	1	−1	$-i$	i	b	$\Gamma_5^+ \times \Gamma_1^-$
L_5^-	Γ_6^-	1	−1	−1	1	$-i$	i	−1	1	1	−1	i	$-i$	b	$\Gamma_6^+ \times \Gamma_1^-$

Magnetic space groups

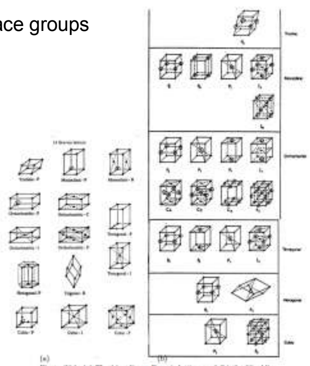

Figure 22.1: (a) The 14 ordinary Bravais lattices and (b) the 22 additional magnetic Bravais lattices. The open circles represent the time reversed sites.

Example

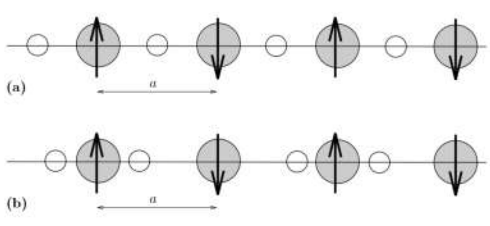

Figure 22.2: Diagram showing a one-dimensional lattice where: (a) the operation $\hat{T}$ is combined with the translation symmetry operation, (b) $\hat{T}$ is not a symmetry operation even if combined with translations.

Two types of group elements:

Unitary operators: A_i

Antiunitary operators: $M_k = TA_k$

$$\begin{aligned} A_i A_{i'} &= A_{i''} \\ A_i M_k &= M_{k'} \\ M_k A_i &= M_{k''} \\ M_{k'} M_{k'} &= A_{i'''} \end{aligned}$$

Types of magnetic point groups

(a) 32 ordinary point groups G' where $\hat{T}$ is not an element

(b) 32 ordinary point groups $G' \otimes \hat{T}$. In these magnetic point groups, all elements A_i of G' are contained together with all elements $\hat{T}A_i$.

(c) 58 point groups G in which half of the elements are $\{A_i\}$ and half are $\{M_k\}$ where $M_k = \hat{T}A_k$ and the $\{A_i, A_k\}$ form an ordinary point group G'. Also $\{A_i\}$ is a subgroup of G'.

total=122