The program NEUTRON: Phonon Selection Rules for neutron and X-ray Inelastic Scattering

J. Manuel Perez-Mato, Mois I. Aroyo, A. Kirov

Universidad del País Vasco
Bilbao

SAM: Modes and selection rules for Infrared and Raman Spectroscopy

NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

Phonon selection rules for neutron and X-ray inelastic scattering

(Mohr et al. PRB 2007)

H: reciprocal lattice vector

$$k = k' + q - H$$

$$Q = k' - k$$

$$Q = H - q$$
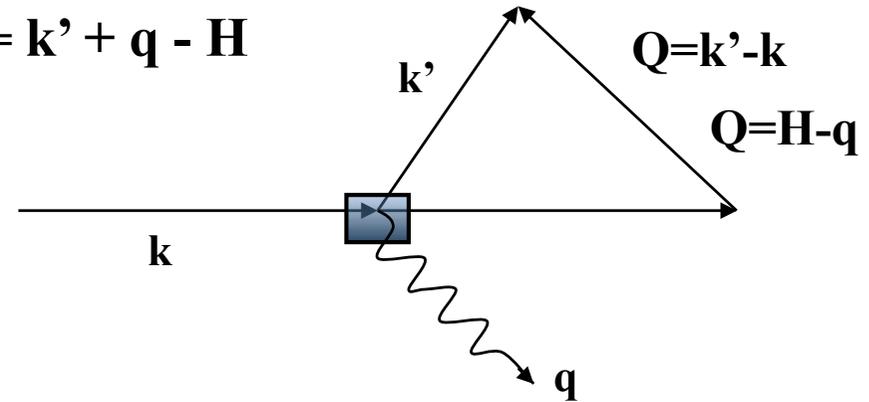
normal mode:

$$u(\mu,T) = A \, (m_\mu)^{-\frac{1}{2}} \, e(\mu|q,j) \, e^{\, iq\cdot(r\mu+T)} + c.c. = A \, \varepsilon(\mu,T|q,j) + c.c.$$

(μ: atoms within cell,   T: lattice translation, j: degeneracy index)

Dynamic structure factor of the mode:

$$F_j(Q) = (1/N) \sum_{\mu,T} b_\mu [\varepsilon(\mu,T|q,j)\cdot Q] \, e^{\, iQ\cdot(r\mu+T)}$$

Intensity from all degenerate modes :

$$I(Q) \sim \sum_j |F_j(Q)|^2 \qquad Q = H - q$$
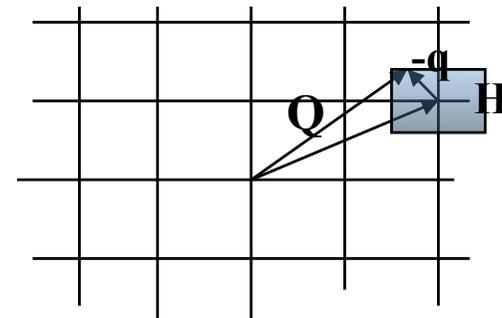
Phonon selection rules for neutron and X-ray inelastic scattering

(PRL 81 (1998) 2462)

$$\mathbf{u}(\mu,\mathbf{T})=A\,\varepsilon(\mu,\mathbf{T}|\mathbf{q},j) + c.c.$$

irrep mode: $D^{q,\tau}$

space group transformation: $(\mathbf{R}|\mathbf{t})$

$$\varepsilon^{tr}(\mu,\mathbf{T}|\mathbf{q},j)=\sum_{i}D^{q,\tau}(\mathbf{R}|\mathbf{t})_{ij}\varepsilon(\mu,\mathbf{T}|\mathbf{q},i)$$

H: reciprocal lattice vector

$$\mathbf{k} = \mathbf{k'} + \mathbf{q} - \mathbf{H}$$

$$\mathbf{Q}=\mathbf{k'}-\mathbf{k}$$

$$\mathbf{Q}=\mathbf{H}-\mathbf{q}$$
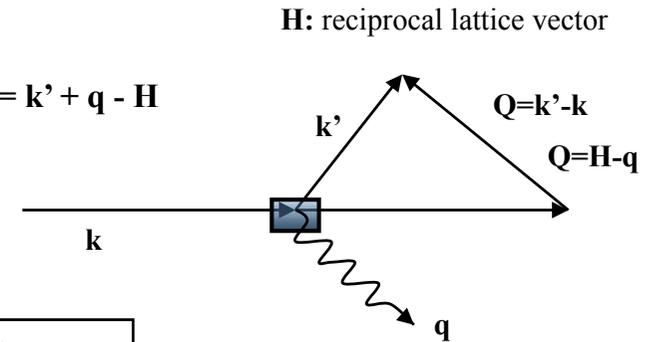
$$F^{tr}_{j}(\mathbf{Q})= (1/N)\sum_{\mu}b_{\mu}[\mathbf{R}\varepsilon(\mu,\mathbf{T}|\mathbf{q},j).\mathbf{Q}]\,e^{\,i\mathbf{Q}.(\mathbf{R}(r\mu+\mathbf{T})+\mathbf{t})}$$

$$F^{tr}_{j}(\mathbf{Q})= (1/N)\sum_{\mu}b_{\mu}[\sum_{i}D^{q,\tau}(\mathbf{R}|\mathbf{t})_{ij}\varepsilon(\mu,\mathbf{T}|\mathbf{q},i).\mathbf{Q}]\,e^{\,i\mathbf{Q}.(\mathbf{R}(r\mu+\mathbf{T})+\mathbf{t})}$$

$$F^{tr}_{j}(\mathbf{RQ})= e^{\,i\mathbf{RQ}.\,\mathbf{t}}\,F_{j}(\mathbf{Q})$$

$$F^{tr}_{j}(\mathbf{Q})= \sum_{i}D^{q,\tau}(\mathbf{R}|\mathbf{t})_{ij}\,F_{i}(\mathbf{Q})$$

> dynamic phonon structure factor transforms according to mode irrep $D^{q,\tau}$

> symmetry property of the phonon dynamic structure factor

$$F_{i}(\mathbf{RQ})=e^{\,i\mathbf{RQ}.\,\mathbf{t}}\sum_{i}D^{q,\tau}(\mathbf{R}|\mathbf{t})^{*}_{ij}\,F_{i}(\mathbf{Q})$$

point group $\mathbf{P^{s}_{Q}}$, all operations $\mathbf{R}$ such that $\mathbf{RQ} = \mathbf{Q}$

$$F_{i}(\mathbf{Q}) = e^{\,i\mathbf{Q}.\,\mathbf{t}}\sum_{j}D^{q,\tau}(\mathbf{R}|\mathbf{t})^{*}_{ij}\,F_{j}(\mathbf{Q})$$

> representation of $\mathbf{P^{s}_{Q}}$

> **Extinction:** For $F_{i}(\mathbf{Q})\neq0$ this representation should contain the identity irrep, otherwise $F_{i}(\mathbf{Q})=0$

NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

Input:

NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

Output:

Inelastic Neutron Scattering Selection Rules for group 34 (*Pnn*2)

```
****************************** Space-group data ******************************

Space group  G34 , number 34
Lattice type : oP

Number of generators : 3

      1                2                3
  1  0  0    0    -1  0  0    0     1  0  0   1/2
  0  1  0    0     0 -1  0    0     0 -1  0   1/2
  0  0  1    0     0  0  1    0     0  0  1   1/2


Translation coset representatives : 4

      1                2                3                4
  1  0  0    0    -1  0  0    0     1  0  0   1/2   -1  0  0   1/2
  0  1  0    0     0 -1  0    0     0 -1  0   1/2    0  1  0   1/2
  0  0  1    0     0  0  1    0     0  0  1   1/2    0  0  1   1/2


****************************** q-vector data ******************************

q-vector GM :
  in primitive basis              :    0.000  0.000  0.000
  in standard dual basis          :    0.000  0.000  0.000

The little group of the q-vector has the following 4
translation coset representatives :

      1                2                3                4
  1  0  0    0    -1  0  0    0     1  0  0   1/2   -1  0  0   1/2
  0  1  0    0     0 -1  0    0     0 -1  0   1/2    0  1  0   1/2
  0  0  1    0     0  0  1    0     0  0  1   1/2    0  0  1   1/2
```

> **"small" irreps of the little group are constructed and labelled:**

```
The little group of the q-vector has  4  allowed irreps.
The matrices, corresponding to all of the little group elements are :

 Irrep (GM)(1) ,  dimension 1
       1              2              3              4
 (1.000,  0.0)  (1.000,  0.0)  (1.000,  0.0)  (1.000,  0.0)


 Irrep (GM)(2) ,  dimension 1
       1              2              3              4
 (1.000,  0.0)  (1.000,  0.0)  (1.000,180.0)  (1.000,180.0)


 Irrep (GM)(3) ,  dimension 1
       1              2              3              4
 (1.000,  0.0)  (1.000,180.0)  (1.000,  0.0)  (1.000,180.0)


 Irrep (GM)(4) ,  dimension 1
       1              2              3              4
 (1.000,  0.0)  (1.000,180.0)  (1.000,180.0)  (1.000,  0.0)
```

NEUTRON: Phonon selection rules for neutron and X-ray inelastic scattering

Output:

```
********************** Q-vector types and extinction rules **********************

General form of Q-vectors: Q = ( h, k, l )

There are 3 types of special Q-vectors.


-----------------------------------------------------------------------
H[1] = ( 0, 0, l )  ,   Q[1] = ( 0, 0, l )
with parameters: l=any

The elements of the little co-group, which leaves Q invariant (strict point group) are:
1 2 3 4

Condition  l=any

For  l = 1

Irrep      Allowed
GM_1         NO
GM_2         YES
GM_3         NO
GM_4         NO

For  l = 2

Irrep      Allowed
GM_1         YES
GM_2         NO
GM_3         NO
GM_4         NO


-----------------------------------------------------------------------
```

Brillouin zones with selection rules for the q chosen

H=(00l)

H=(h0l)

```
-----------------------------------------------------------------------
H[2] = ( h, 0, l )  ,   Q[2] = ( h, 0, l )
with parameters: h=any, l=any

The elements of the little co-group, which leaves Q i
1 3

Condition  h=any, l=any

For  h = 1 ,   l = 1

Irrep      Allowed
GM_1         YES
GM_2         NO
GM_3         YES
GM_4         NO

For  h = 1 ,   l = 2

Irrep      Allowed
GM_1         NO
GM_2         YES
GM_3         NO
GM_4         YES
```

h+l=even

h+l=odd

l=odd

l=even

Example: Phonon selection rules for the line Σ(α,0,0) in Pnn2
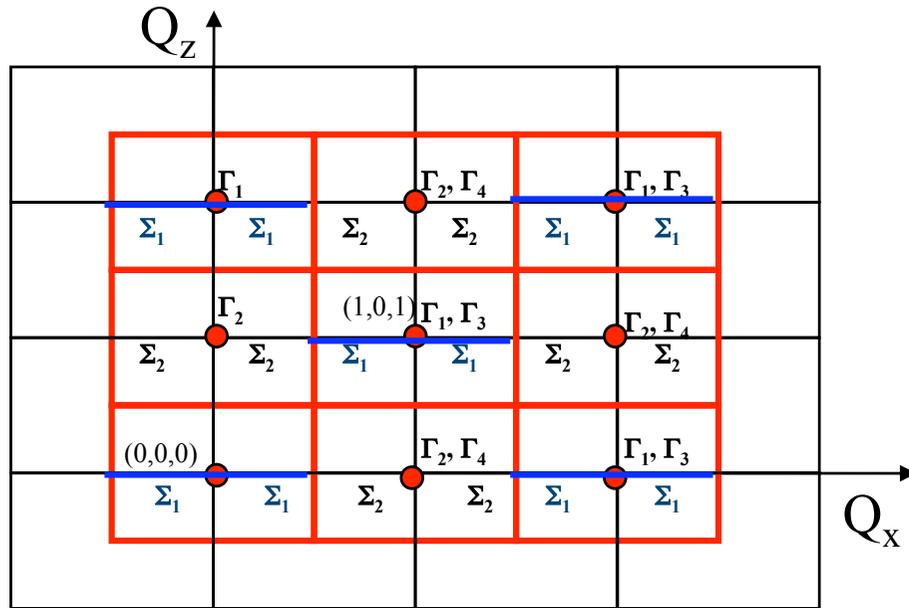
		q=(0 0 0)	q=(α 0 0)
H	condition	allowed	Allow.
(0 0 1)	l -even	Γ_1	Σ_1
	l - odd	Γ_2	Σ_2
(h 0 l)	h+l -even	Γ_1 , Γ_3	Σ_1
	h+l -odd	Γ_2 , Γ_4	Σ_2
(0 k l)	k+l -even	Γ_1 , Γ_4	No restric.
	k+l -odd	Γ_2 , Γ_3	
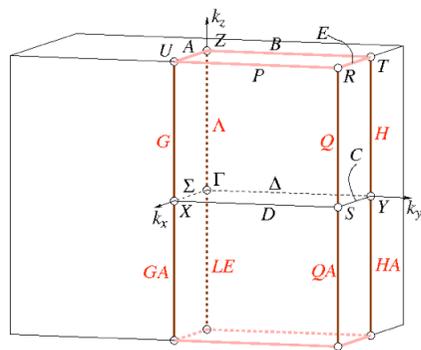
Brillouin zone Pnn2
(KVEC)

irreps:

q=(0 0 0)

	E	m_x	m_y	2_z
Γ_1	1	1	1	1
Γ_2	1	-1	-1	1
Γ_3	1	-1	1	-1
Γ_4	1	1	-1	-1

q=(α 0 0)

	E	m_y
Σ_1	1	1
Σ_2	1	-1

Example: Phonon selection rules for the line Σ(α,0,0) in Pnn2
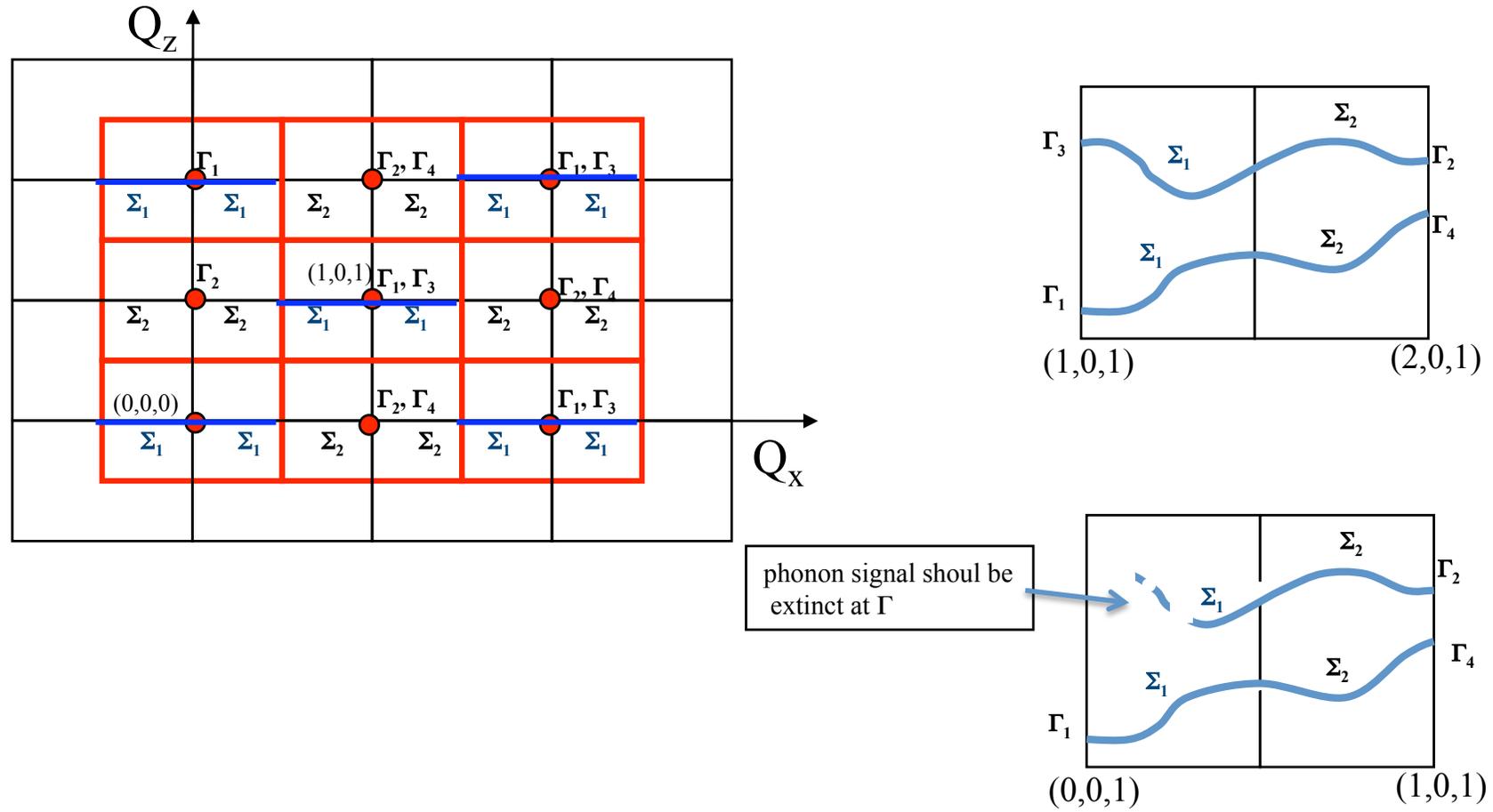
Example: Phonon selection rules for Pn-3m

line Γ(0,0,0) - example
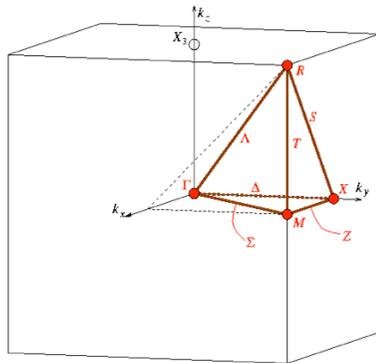
```
-----------------------------------------------------------------------------------

H[2] = ( h, h, h )   ,    Q[2] = ( h, h, h )
with parameters: h=any

The elements of the little co-group, which leaves Q invariant (strict point group) are:
1 5 9 38 44 47

Condition   h=any

For   h = 1

Irrep         Allowed
GM_1            YES
GM_2            NO
GM_3            NO
GM_4            YES
GM_5            NO
GM_6            NO
GM_7            NO
GM_8            YES
GM_9            YES
GM_10           NO


-----------------------------------------------------------------------------------
```

line Δ(α,0,0) - example

```
-----------------------------------------------------------------------------------

H[3] = ( h, k, k )   ,    Q[3] = ( h - 0.21, k, k )
with parameters: h=any, k=any

The elements of the little co-group, which leaves Q invariant (strict point group) are:
1 7

Condition   h=any, k=any

For   h = 1 ,   k = 1

Irrep         Allowed
DT_1            YES
DT_2            NO
DT_3            NO
DT_4            YES
DT_5            YES


*********************************** END ***********************************
```

Phonon/modes selection rules also present in diffuse scattering

NEUTRON can also be used to interpret patterns of diffuse scattering

ThAsSe (Withers et al., JSSC (2004)
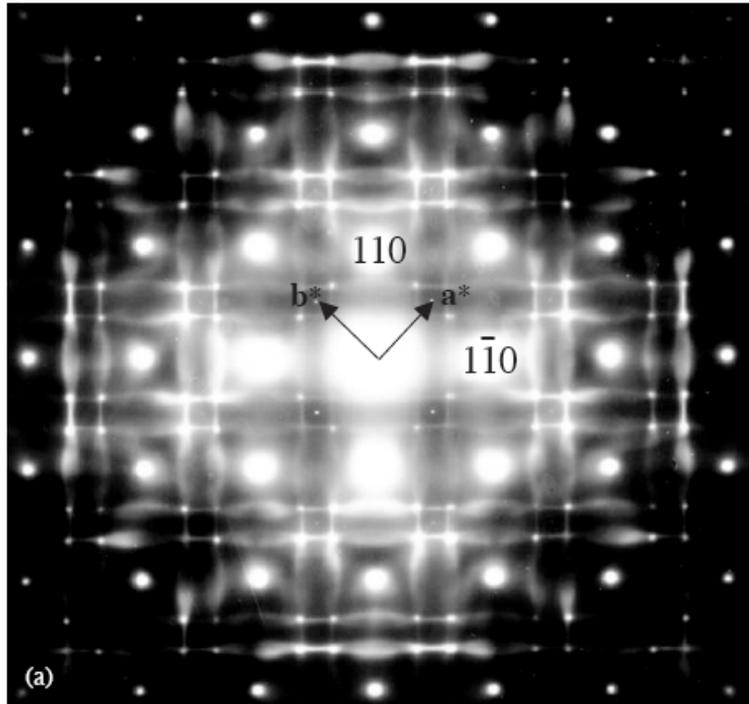
P4/nmm

Diffuse streaks: $(h,k,0) + \mathbf{q}$, $\mathbf{q} = (\alpha,\beta,0)$

$h+k = odd$

program NEUTRON:

$q = (\alpha,\beta,0)$ - 2 irreps: D_1, D_2

$h+k = even$ ---- D_1 allowed
$h+k = odd$ ---- D_2 allowed