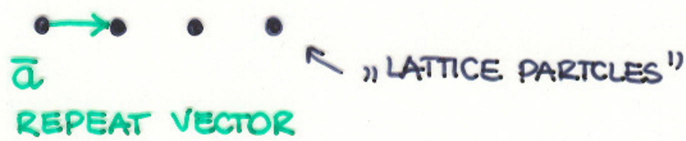
CRYSTALS

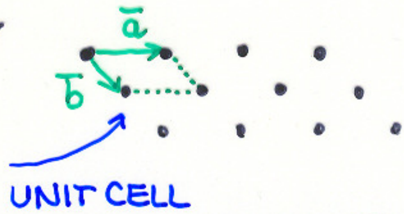
TRANSLATIONS – SPECIFIC SYMMETRY OPERATION

A PROPERTY AT THE ATOMIC LEVEL („MICROSCOPIC SYMMETRY"), NOT SYMMETRY OF CRYSTAL SHAPES

1-D TRANSLATIONS: A ROW



2-D TRANSLATIONS: A NET



TRANSLATION (REPEAT) OF UNIT CELL GENERATES THE WHOLE CRYSTAL LATTICE

SYMMETRY OPERATIONS

POINT GROUPS

$\{\alpha \mid 0\}$

„ROTATIONS"

ELEMENTS OF POINT GROUPS

$+$

$\{0 \mid \vec{R}\}$ ALL TRANSLATIONS (INFINITE NUMBER)

$\vec{R} = l_1\bar{a}_1 + l_2\bar{a}_2 + l_3\bar{a}_3$

$\{l_1, l_2, l_3\}$ – INTEGERS

$\{\bar{a}_1, \bar{a}_2, \bar{a}_3\}$ BASIC VECTORS

SPACE GROUPS

A GENERAL ELEMENT $\{\check{\alpha} \mid \bar{R}\}\,\bar{r} \Rightarrow \bar{r}' = \check{\alpha}\bar{r} + \bar{R}$ SYMMETRY OPERATION

TO EACH $\{\check{\alpha} \mid \bar{R}\}$ A LINEAR OPERATOR $P_{\{\check{\alpha} \mid \bar{R}\}}$ IS ASSIGNED

(REPRESENTATION BASED ON ISOMORPHISM)

$\{0|\bar{R}\}$: $P_{\{0|\bar{R}\}} \equiv T_{\bar{R}}$ PURE LATTICE TRANSLATION

$\{T_{\bar{R}}\}$ FOR <u>ALL</u> $\bar{R}$ = SUBGROUP OF THE SPACE GROUP

PROPERTIES OF THIS GROUP ARE THE MOST IMPORTANT IN THE SOLID STATE THEORY!

(*) $T_{\bar{R}} T_{\bar{R}'} = T_{\bar{R}'} T_{\bar{R}}$ ABELIAN GROUP

ALL ELEMENTS COMMUTE

$$\{0|\bar{R}\}\{0|\bar{R}'\}\bar{r} = \{0|\bar{R}\}(\bar{r}+\bar{R}') = (\bar{r}+\bar{R}'+\bar{R}) = (\bar{r}+\bar{R}+\bar{R}') = \{0|\bar{R}'\}(\bar{r}+\bar{R}) = \{0|\bar{R}'\}\{0|\bar{R}\}\bar{r}$$

(*) $T_{\bar{R}} T_{\bar{R}'} = T_{\bar{R}+\bar{R}'}$

IN ORDER TO GROUP THE ELEMENTS INTO CLASSES:

$$T_{\bar{R}'}^{-1} T_{\bar{R}} T_{\bar{R}'} = ?$$

$$T_{\bar{R}'}^{-1} T_{\bar{R}} T_{\bar{R}'} = \underbrace{T_{\bar{R}'}^{-1} T_{\bar{R}'}}_{\hat{E}} T_{\bar{R}} = T_{\bar{R}}$$

FOR ALL ELEMENTS OF THE GROUP OF PURE TRANSLATIONS!

CONJUGATED WITH ITSELF

CONCLUSION: <u>EACH ELEMENT FORMS A SEPARATE CLASS!</u>

CONSEQUENCES:

1°. THE NUMBER OF CLASSES = h (ORDER OF THE GROUP),

2°. THE NUMBER OF REPRESENTATIONS (IRREDUCIBLE) = NUMBER OF CLASSES = h,

3° THE SUM OF THE SQUERES OF THE DIMENSIONS OF IRREDUCIBLE REPRESENTATIONS

$$\underbrace{r_1^2 + r_2^2 + \dots}_{h \text{ ELEMENTS}} = h \quad \Rightarrow \quad r_1 = r_2 = \dots = 1$$

ALL IRREDUCIBLE REPRESENTATIONS OF $\{T_{\bar{R}}\}$ ARE

ONE-DIMENSIONAL

$$T_{\bar{R}}\,\psi(\bar{r}) = C(\bar{R})\,\psi(\bar{r})$$ $C(\bar{R})$ = NUMBER

UNITARY TRANSFORMATION $\Rightarrow |C(\bar{R})|^2 = 1$

$$T_{\bar{R}}T_{\bar{R}'} = T_{\bar{R}+\bar{R}'} \Rightarrow \quad C(\bar{R})C(\bar{R}') = C(\bar{R}+\bar{R}')$$

THE ONLY REALIZATION:

$$C(\bar{R}) = e^{i\bar{k}\bar{R}}$$ $\bar{k}$ – REAL VECTOR

$$T_{\bar{R}}\,\psi(\bar{r}) = \underbrace{e^{i\bar{k}\bar{R}}}_{\text{EIGENVALUE}}\,\psi(\bar{r})$$

EIGENFUNCTION

$\psi(\bar{r}) \equiv \psi_{\bar{k}}(\bar{r})$

$$\boxed{T_{\bar{R}}\,\psi_{\bar{k}}(\bar{r}) = e^{i\bar{k}\bar{R}}\,\psi_{\bar{k}}(\bar{r})}$$ BLOCH THEOREM

$T_{\bar{R}}$ – SYMMETRY OPERATION

$[H, T_{\bar{R}}] = 0 \quad \Rightarrow \quad H\psi_{\bar{k}} = E_{\bar{k}}\psi_{\bar{k}}$

FOR ALL $\bar{R}$

$\vec{k}$ = WAVE VECTOR DEFINED WITHIN THE RECIPROCAL LATTICE, RESTRICTED TO THE FIRST BRILLOUIN ZONE, PSEUDO-MOMENTUM OF $\bar{e}$ OR MOMENTUM OF PSEUDO PARTICLE (" CRYSTAL ELECTRON): $\bar{\nabla}\psi_{\bar{k}} = ?$

BLOCH'S FUNCTION

$$\psi_{\bar{k}}(\bar{r}) = u_{\bar{k}}(\bar{r})\,e^{i\bar{k}\bar{r}}$$

PLANE WAVE MODULATED BY A PERIODIC FUNCTION

$$u_{\bar{k}}(\bar{r}+\bar{R}) = u_{\bar{k}}(\bar{r})$$

CONSEQUENCES.....

THE EIGENFUNCTIONS OF H (ENERGY STATES) THAT DESCRIBES THE ENERGY OF $\bar{e}$ IN CRYSTALS ARE IDENTIFIED BY THE IRREDUCIBLE REPRESENTATIONS OF THE GROUP OF PURE TRANSLATIONS ($\equiv$ SUBGROUP OF A SPACE GROUP)

IS ANY INFLUENCE OF PERIODICITY UPON THE ENERGY STRUCTURE OF $\bar{e}$ IN CRYSTALS?