PC5203 Advanced Solid State Physics

Weeks 1-3, due Monday 30 Aug 2021

[main concepts to cover: group theory, representations of group as unitary matrices, faithful, unfaith, reducible and irreducible representations, character table, quantum wave functions as basis of presentations, Mulliken symbol for irreducible representation.]

1. (a) For the symmetry group of triangle, C_{3v}, work out all the matrices D(A) for the atom site representation (3x3) $\Gamma^{a.s.}$ and the 2D vector representation (2x2) Γ(x,y), and verify that $A^2=B^2=C^2=E$, $D^3 = F^3 =E$, $F^2 = D$, FA=B, for both representations [See also slide 9 of week 1]

   (b) Compute the characters $\chi(\mathrm{A})$ of each class in (a), put into a table together with the original character table of all irreducible representations.

   (c) Which of these 5 representations, A_1, A_2, E, $\Gamma^{a.s}$, and Γ(x,y) on the table in (b) are faithful representations?

   (d) Are the atom site $\Gamma^{a.s.}$ and vector Γ(x,y) irreducible representations? If yes, which one according to Mulliken symbol. If not, what irreducible representations they can be decomposed into as a direct sum?

2. The space group of a 2D graphene is P6mm. P stand for primitive, 6 means there is 6-fold symmetry axis, mm means there are two types of mirror reflections. Let C_6 denote 60-degree rotation. σ denotes vertical mirror reflection pass through the origin (see figure on slide 12 of week 1). $\boldsymbol{R}$ is lattice translation. (a) Express the two point group operations as 2 by 2 matrices, and $\boldsymbol{R}$ as 2D vector (x, y) in terms of the lattice constant $a = |\boldsymbol{a}_1| = |\boldsymbol{a}_2|$. (b) The operation of vertical glide reflection (the long vertical blue dotted line shown on slide 12) is to translate vertically by appropriate amount and then reflect. Write this as an equation $(x, y) \rightarrow (x', y')$, i.e., give the primed coordinates representing this operation. (c) Since graphene is symmorphic, all space group elements can be written as $\{\alpha|\boldsymbol{R}\}$ where α is an element in C_{6v} and $\boldsymbol{R}$ is the translation by the lattice vector (see slide 4) so that a point at $\boldsymbol{x}$ is moved to $\alpha\boldsymbol{x} + \boldsymbol{R}$. Find the $\{\alpha|\boldsymbol{R}\}$ such that the net effect is the vertical glide reflection in (b).

3. Benzene molecule has a C_{6v} symmetry (disregard the z direction). Using a tight-binding hopping Hamiltonian of 6 sites $i = 1, 2, 3, \ldots, 6$ of the form $H_{ij} = -t$, if $(i-j) = \pm 1$

mod 6, and 0 otherwise (i.e., periodic boundary condition on a ring of six sites). (a) determine the eigen energies E_n of the Hamiltonian H (Hint: try plane wave form $\Psi \propto e^{ikj}$ of the solution, here *j* label the sites; determine *k* using periodic boundary condition). (b) Classify the six eigenstates Ψ_n according to the irreducible representation of C_{6v} and assign the appropriate Mulliken symbol to them.