Condensed Matter II

Problem set #7

Spring 2023

1 Donor states in Si

The conduction band of Silicium exhibits six equivalent minima in the direction Δ in the first Brillouin zone. The electronic state vectors in such directions are designated by the following symbols:

- $|x\rangle$ for the minimum in direction [100]
- $|y\rangle$ for the minimum in direction [010]
- $|z\rangle$ for the minimum in direction [001]
- $|\bar{x}\rangle$ for the minimum in direction $[\bar{1}00]$
- $|\bar{y}\rangle$ for the minimum in direction $[0\bar{1}0]$
- $|\bar{z}\rangle$ for the minimum in direction $[00\bar{1}]$

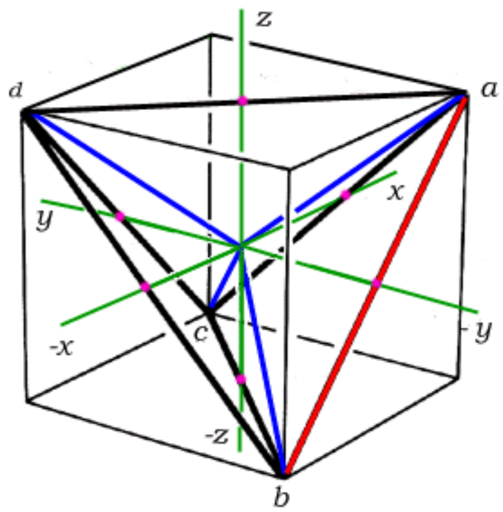

Figure 1: Regular tetrahedron with vertices Si atoms on the a, b, c, d sites. In the middle of the tetrahedron is a donor atom.

A donor atom is located at the center of a regular tetrahedron as indicated in Fig 1. As a reminder, the symmetry of the tetrahedraon is T_d, of order 24, with elements:

- E (identity)
- 8 rotations C_3 about the diagonals of a cube.
- 3 rotations C_2 about axes x, y, z.
- 6 improper rotations S_4 about axis x, y, z (rotations of angle $\pi/2$ followed by a reflection in a plane perpendicular to the axis of rotation).
- 6 reflections σ_d in planes containing one edge and the center of the tetrahedron.

1.1 Questions

(i) Apply a symmetry operation of each class of the T_d group to the six dimensional vector $\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix}$

(ii) Use the previous result to establish the character table of the six-dimensional representation R_6 of the group T_d.

(iii) Using the previously established (Cf Problem Set #3) character table of the T_d group, decompose R_6 into its irreducible components.

(iv) Verify that the following vector states are bases of the corresponding irreducible representations:

- $A_1 : \dfrac{|x\rangle + |y\rangle + |z\rangle + |\bar{x}\rangle + |\bar{y}\rangle + |\bar{z}\rangle}{\sqrt{6}}$
- $E : \dfrac{|x\rangle - |y\rangle + |\bar{x}\rangle - |\bar{y}\rangle}{2}, \dfrac{|x\rangle + |y\rangle - 2\,|z\rangle + |\bar{x}\rangle + |\bar{y}\rangle - 2\,|\bar{z}\rangle}{\sqrt{12}}$
- $T_2 : \dfrac{|x\rangle - |\bar{x}\rangle}{\sqrt{2}}, \dfrac{|y\rangle - |\bar{y}\rangle}{\sqrt{2}}, \dfrac{|z\rangle - |\bar{z}\rangle}{\sqrt{2}}$