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Chapter 16

Notes on Line Graphs

16.1 Line graphs: Kagomé and Checkerboard Lattices

A *line graph* is constructed by taking a given graph and associating a site to every link in the graph. Two sites are connected if their corresponding links share a vertex in the original graph. To every closed loop of even perimeter on the original graph there corresponds an eigenstate of the adjacency matrix of the line graph, with eigenvalue $\lambda = 2$, provided those closed loops are all *even-membered*.

16.1.1 Kagomé lattice

The Kagomé lattice, depicted in fig. 16.1, is a triangular Bravais lattice with a three element basis. It is the line graph of the honeycomb lattice. Choosing primitive direct lattice vectors $\mathbf{a}_1 = \hat{x}$ and $\mathbf{a}_2 = \frac{1}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}$, we then write

$$\begin{pmatrix} a_R \\ b_R \\ c_R \end{pmatrix} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} \begin{pmatrix} a_{\mathbf{k}} \\ e^{\frac{i}{2}\mathbf{k}\cdot\mathbf{a}_1} b_{\mathbf{k}} \\ e^{\frac{i}{2}\mathbf{k}\cdot\mathbf{a}_2} c_{\mathbf{k}} \end{pmatrix}. \quad (16.1)$$

The basis vectors here are 0 , $\frac{1}{2}\mathbf{a}_1$, and $\frac{1}{2}\mathbf{a}_2$.

With $\theta_i = \mathbf{k} \cdot \mathbf{a}_i$, we then have the Hamiltonian

$$H_{\mathbf{k}} = - \begin{pmatrix} 0 & 2tc_1 & 2tc_2 \\ 2tc_1 & 0 & 2tc_{12} \\ 2tc_2 & 2tc_{12} & 0 \end{pmatrix}, \quad (16.2)$$

where as before $c_i = \cos \frac{1}{2}\theta_i$ and $c_{ij} = \cos \frac{1}{2}(\theta_i - \theta_j)$. The eigenvalues are

$$E_{1,2} = -t \pm t\sqrt{3 + 2\cos\theta_1 + 2\cos\theta_2 + 2\cos(\theta_1 - \theta_2)} \quad (16.3)$$

and

$$E_3 = +2t. \quad (16.4)$$

Thus, there is a lower band with energies in the interval $E_1 \in [-4t, -t]$, a middle band with $E_2 \in [-t, +2t]$, and a flat upper band with $E_3 = +2t$.

16.1.2 Checkerboard lattice

The checkerboard lattice, also known as the planar pyrochlore structure, is depicted in fig. 16.2. It is the line graph of the square lattice. It may be represented as an underlying square lattice with primitive direct lattice vectors $\mathbf{a}_1 = \hat{x} - \hat{y}$ and $\mathbf{a}_2 = \hat{x} + \hat{y}$, with a two element basis 0 and \hat{x} .

$$\begin{pmatrix} a_R \\ b_R \end{pmatrix} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}} \begin{pmatrix} a_{\mathbf{k}} \\ e^{i\frac{1}{2}\mathbf{k}\cdot\hat{x}} b_{\mathbf{k}} \end{pmatrix}. \quad (16.5)$$

If the hoppings are t along $\pm\hat{x}$ and $\pm\hat{y}$, and t' along $\pm\mathbf{a}_1$ and $\pm\mathbf{a}_2$, then the Hamiltonian is

$$H_{\mathbf{k}} = - \begin{pmatrix} 2t' \cos\theta_2 & 4t \cos(\frac{1}{2}\theta_1) \cos(\frac{1}{2}\theta_2) \\ 4t \cos(\frac{1}{2}\theta_1) \cos(\frac{1}{2}\theta_2) & 2t' \cos\theta_1 \end{pmatrix}, \quad (16.6)$$

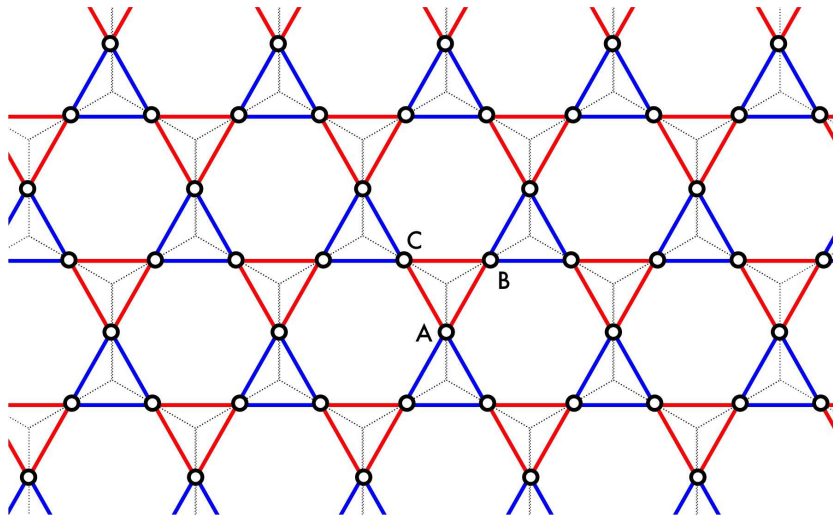


Figure 16.1: The Kagomé lattice, which is a triangular Bravais lattice with a three element basis (A,B,C). The Kagomé lattice is the line graph of a honeycomb lattice.

with eigenvalues

$$E_{1,2} = -t'(\cos \theta_1 + \cos \theta_2) \pm \sqrt{(t' \cos \theta_1 - t' \cos \theta_2)^2 + 4t^2(1 + \cos \theta_1)(1 + \cos \theta_2)}. \quad (16.7)$$

When $t = t'$ this simplifies to

$$E_1 = -2t(1 + \cos \theta_1 + \cos \theta_2) \quad , \quad E_2 = +2t. \quad (16.8)$$

Once again, as in the Kagomé and pyrochlore lattices, the top band is flat.

16.1.3 Square-octagon lattice line graph

The line graph of the square-octagon lattice is shown in Fig. 16.3. The Hamiltonian is

$$H_k = - \begin{pmatrix} 0 & t_1 & t_2 e^{-ik_x} & 0 & t_2 e^{-ik_y} & t_1 \\ t_1 & 0 & t_2 & t_1 & t_2 e^{-ik_y} & 0 \\ t_2 e^{ik_x} & t_2 & 0 & t_2 & 0 & t_2 e^{ik_x} \\ 0 & t_1 & t_2 & 0 & t_2 & t_1 \\ t_2 e^{ik_y} & t_2 e^{ik_y} & 0 & t_2 & 0 & t_2 \\ t_1 & 0 & t_2 e^{-ik_x} & t_1 & t_2 & 0 \end{pmatrix}, \quad (16.9)$$

where t_1 is the hopping along the blue links and t_2 the hopping along the red links. When $t_1 \neq t_2$, the adjacency matrix has a flat band at $\lambda = 2t_1$. When $t_1 = t_2$, the flat band is doubly degenerate.

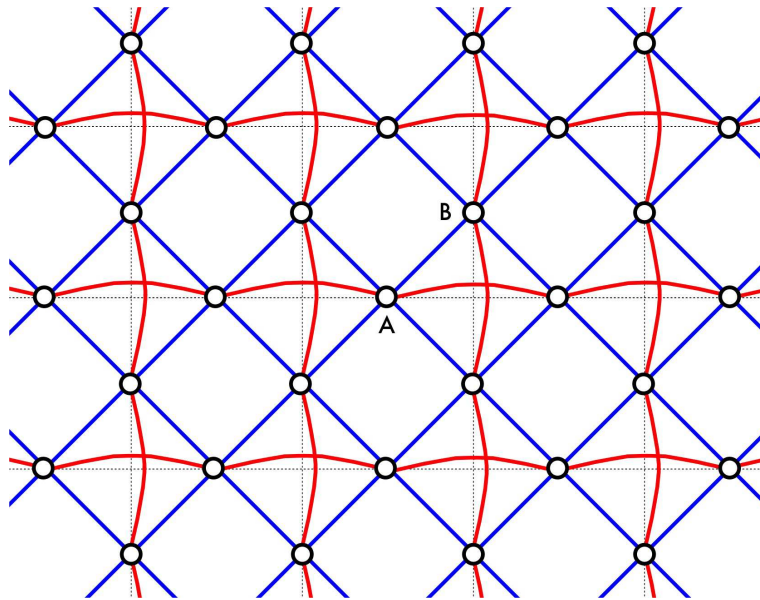


Figure 16.2: The checkerboard (planar pyrochlore) lattice, which is a square lattice with a two element basis (A,B). The checkerboard lattice is the line graph of the square lattice.

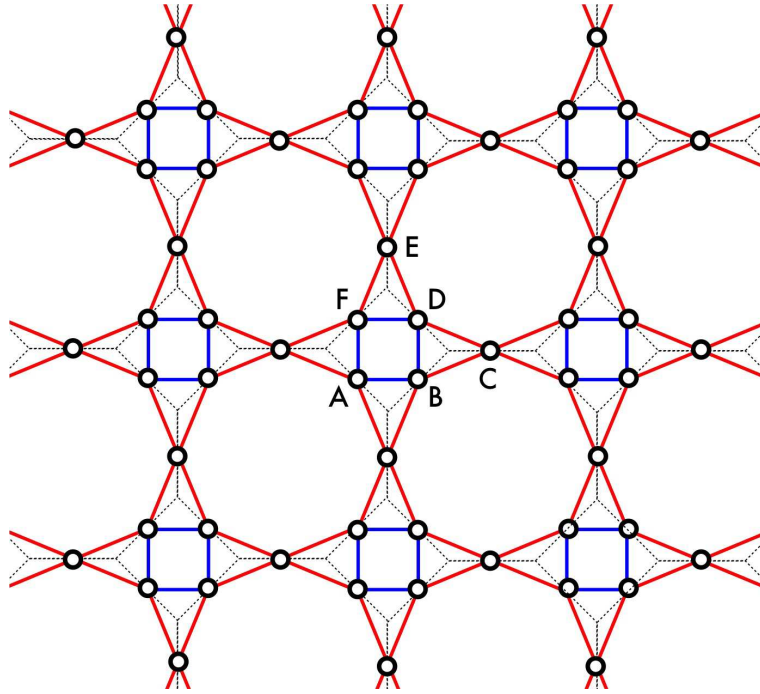


Figure 16.3: This fourfold coordinated lattice is the line graph of the square-octagon lattice. The hopping along the blue links is t_1 and that along the red links is t_2 .

16.2 Pyrochlore Lattice

The pyrochlore lattice (fig. 16.5) is a sixfold-coordinated structure whose underlying Bravais lattice is FCC, with a four element basis. It is effectively described as a diamond lattice of ‘corner-sharing tetrahedra’. Recall that diamond is FCC with a two element basis. It can be constructed as the line graph of the diamond lattice.

To apprehend the geometry better, consider the sketch in fig. 16.6. Let the center of the cube, indicated by the yellow star, be located at the origin $(0, 0, 0)$. Then the four corners of the tetrahedron are located as

$$\begin{aligned} \mathbf{A} &= \frac{d}{2}(+1, -1, +1) & \mathbf{C} &= \frac{d}{2}(+1, +1, -1) \\ \mathbf{B} &= \frac{d}{2}(-1, +1, +1) & \mathbf{D} &= \frac{d}{2}(-1, -1, -1). \end{aligned}$$

There are two species of tetrahedra in the pyrochlore lattice, which we call α and β (see figure 16.7). We identify the tetrahedron depicted in fig. 16.6 as an α -tetrahedron. The centers of the four neighboring β -tetrahedra are then located at $2\mathbf{A}$, $2\mathbf{B}$, $2\mathbf{C}$, and $2\mathbf{D}$. That is, to move from the center of an α -tetrahedron to the center of a neighboring β -tetrahedron, we displace by one of these four vectors. This set is not invariant under inversion. To move from the center of a β -tetrahedron to the center of a neighboring α -tetrahedron, we displace by the negative of one of these four vectors.

Thus, the twelve nearest neighbor displacements on the underlying FCC Bravais lattice are given by $2(\mathbf{A} - \mathbf{B})$, $2(\mathbf{A} - \mathbf{C})$, etc., since we move from (the center of) one α -tetrahedron to another. These twelve vectors may be written as

$$2\mathbf{A} - 2\mathbf{B} = \frac{a}{\sqrt{2}} (+1, -1, 0) = -\mathbf{a}_1 + \mathbf{a}_2 \quad (16.10)$$

$$2\mathbf{A} - 2\mathbf{C} = \frac{a}{\sqrt{2}} (0, -1, +1) = \mathbf{a}_2 - \mathbf{a}_3$$

$$2\mathbf{A} - 2\mathbf{D} = \frac{a}{\sqrt{2}} (+1, 0, +1) = \mathbf{a}_2$$

$$2\mathbf{B} - 2\mathbf{C} = \frac{a}{\sqrt{2}} (-1, 0, +1) = \mathbf{a}_1 - \mathbf{a}_3$$

$$2\mathbf{B} - 2\mathbf{D} = \frac{a}{\sqrt{2}} (0, +1, +1) = \mathbf{a}_1$$

$$2\mathbf{C} - 2\mathbf{D} = \frac{a}{\sqrt{2}} (+1, +1, 0) = \mathbf{a}_3 \quad (16.11)$$

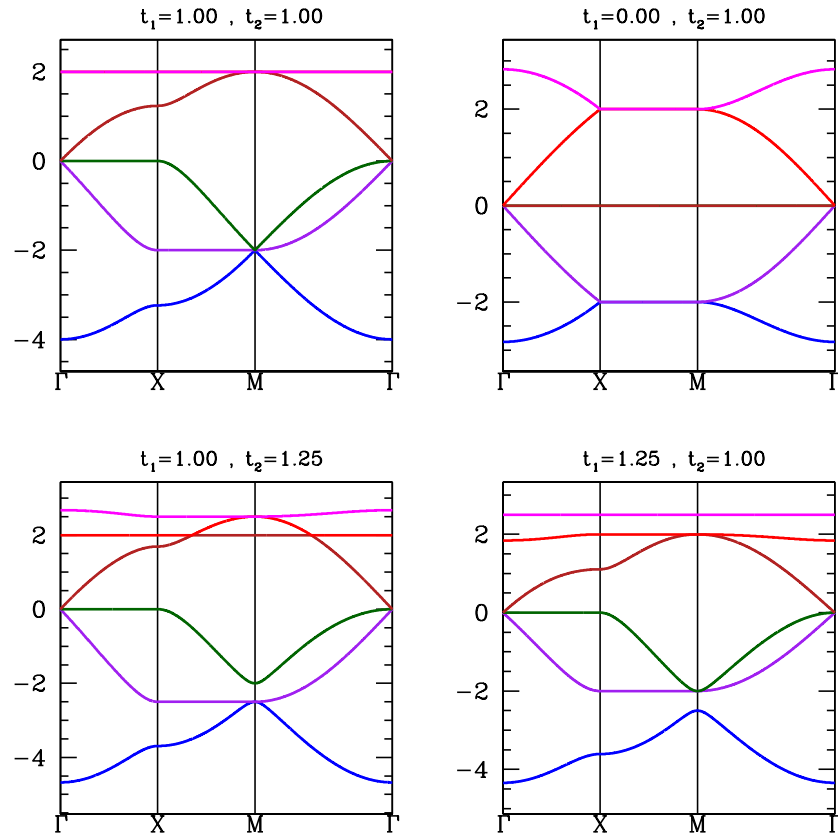


Figure 16.4: Energy bands for the line graph of the square-octagon lattice.

and their negatives, where $a = 2\sqrt{2}d$ is the FCC lattice constant. Here

$$\mathbf{a}_1 = \frac{a}{\sqrt{2}}(0, 1, 1) \quad \mathbf{a}_2 = \frac{a}{\sqrt{2}}(1, 0, 1) \quad \mathbf{a}_3 = \frac{a}{\sqrt{2}}(1, 1, 0) \quad (16.12)$$

are primitive FCC direct lattice basis vectors. Note $a = 2b$ relates the side length of the tetrahedra to the FCC lattice constant. The center of any α -tetrahedron is then located at

$$\mathbf{R} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3, \quad (16.13)$$

and the four basis vectors are $s_{1,2,3,4} = \{\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}\}$, *i.e.*

$$\begin{aligned} \mathbf{s}_1 &= \frac{a}{4\sqrt{2}}(1, -1, 1) & \mathbf{s}_3 &= \frac{a}{4\sqrt{2}}(1, 1, -1) \\ \mathbf{s}_2 &= \frac{a}{4\sqrt{2}}(-1, 1, 1) & \mathbf{s}_4 &= \frac{a}{4\sqrt{2}}(-1, -1, -1). \end{aligned} \quad (16.14)$$

The reciprocal lattice is BCC, with primitive vectors

$$\mathbf{b}_1 = \frac{\sqrt{2}\pi}{a}(-1, 1, 1) \quad , \quad \mathbf{b}_2 = \frac{\sqrt{2}\pi}{a}(1, -1, 1) \quad , \quad \mathbf{b}_3 = \frac{\sqrt{2}\pi}{a}(1, 1, -1), \quad (16.15)$$

which satisfy $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi \delta_{ij}$.

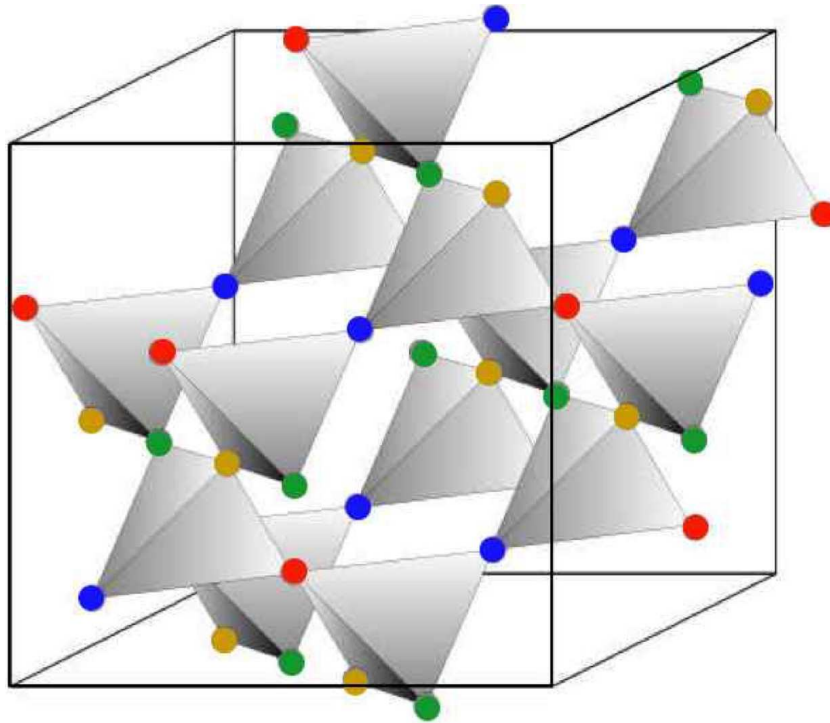


Figure 16.5: The pyrochlore lattice is an FCC Bravais lattice with a four element basis.

16.2.1 Adjacency Matrix

Let us label each vertex on the pyrochlore lattice by a Bravais lattice site $\mathbf{R}_{m_1, m_2, m_3}$ (*i.e.* the center of an α -tetrahedron) and by a sublattice index, with $A \equiv 1, B \equiv 2, C \equiv 3, D \equiv 4$. The adjacency matrix is

$$A_{ij}(\mathbf{R}) = \begin{pmatrix} 0 & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_2 - a_1} & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_2 - a_3} & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_2} \\ \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_1 - a_2} & 0 & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_1 - a_3} & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_1} \\ \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_3 - a_2} & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_3 - a_1} & 0 & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, a_3} \\ \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, -a_2} & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, -a_1} & \delta_{\mathbf{R},0} + \delta_{\mathbf{R}, -a_3} & 0 \end{pmatrix}. \quad (16.16)$$

The definition of the adjacency matrix is that $A_{ij}(\mathbf{R}) = 1$ if sites s_i and $\mathbf{R} + s_j$ are nearest neighbors.

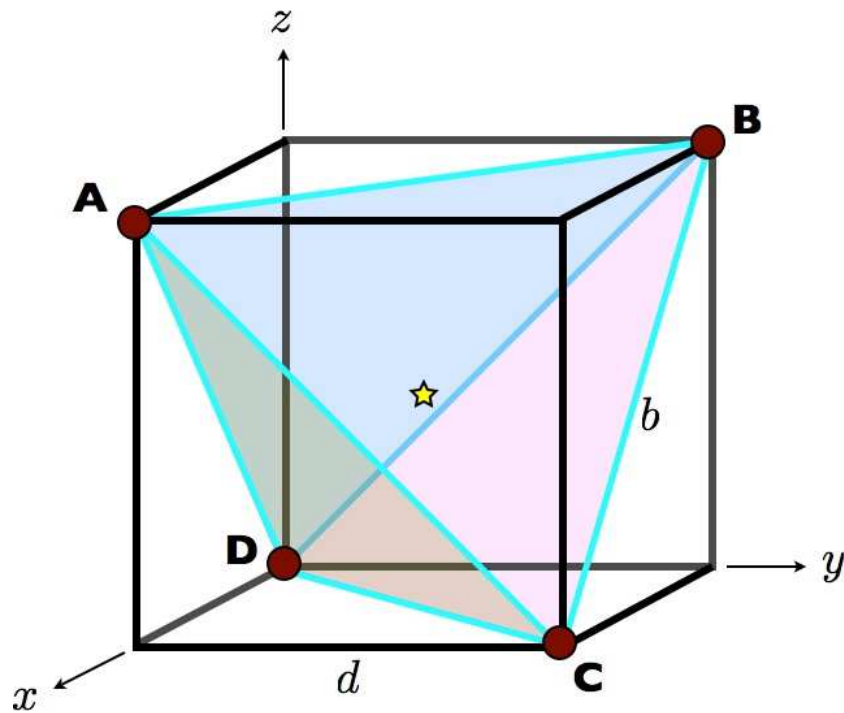


Figure 16.6: A cube of side length d , containing a tetrahedron of side length $b = \sqrt{2}d$. The origin of coordinates is located at the yellow star, which lies at the geometric center of the cube.

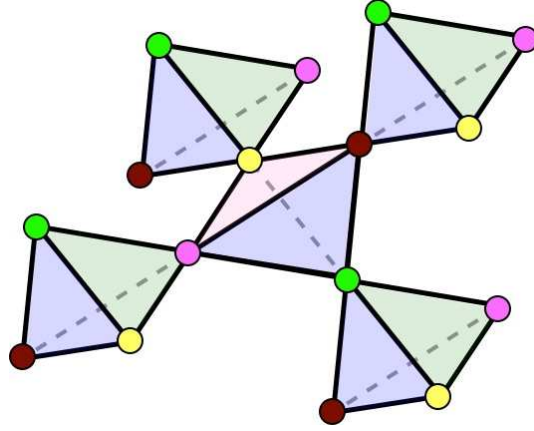


Figure 16.7: The α and β tetrahedra are related by inversion. The colors of the sites show the sublattice structure.

The Fourier transform of the adjacency matrix is

$$\hat{A}_{ij}(\mathbf{k}) = \sum_{\mathbf{R}} A_{ij}(\mathbf{R}) e^{i\mathbf{k}\cdot\mathbf{R}} \quad (16.17)$$

$$= \begin{pmatrix} 0 & 1 + e^{i(\theta_2 - \theta_1)} & 1 + e^{i(\theta_2 - \theta_3)} & 1 + e^{i\theta_2} \\ 1 + e^{i(\theta_1 - \theta_2)} & 0 & 1 + e^{i(\theta_1 - \theta_3)} & 1 + e^{i\theta_1} \\ 1 + e^{i(\theta_3 - \theta_2)} & 1 + e^{i(\theta_3 - \theta_1)} & 0 & 1 + e^{i\theta_3} \\ 1 + e^{-i\theta_2} & 1 + e^{-i\theta_1} & 1 + e^{-i\theta_3} & 0 \end{pmatrix}, \quad (16.18)$$

where we define

$$\mathbf{k} \equiv \frac{\theta_1 \mathbf{b}_1}{2\pi} + \frac{\theta_2 \mathbf{b}_2}{2\pi} + \frac{\theta_3 \mathbf{b}_3}{2\pi}, \quad (16.19)$$

so that

$$\mathbf{k} \cdot \mathbf{R}_{m_1, m_2, m_3} = m_1 \theta_1 + m_2 \theta_2 + m_3 \theta_3. \quad (16.20)$$

Note that the unitary transformation,

$$U = \begin{pmatrix} e^{i\theta_2/2} & 0 & 0 & 0 \\ 0 & e^{i\theta_1/2} & 0 & 0 \\ 0 & 0 & e^{i\theta_3/2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (16.21)$$

has the effect

$$U^\dagger \hat{A}_{ij}(\mathbf{k}) U = 2 \begin{pmatrix} 0 & c_{12} & c_{23} & c_2 \\ c_{12} & 0 & c_{13} & c_1 \\ c_{23} & c_{13} & 0 & c_3 \\ c_2 & c_1 & c_3 & 0 \end{pmatrix}, \quad (16.22)$$

where $c_i = \cos \frac{1}{2}\theta_i$ and $c_{ij} = \cos \frac{1}{2}(\theta_i - \theta_j)$.

The characteristic polynomial is found to be

$$\begin{aligned} P(\lambda) &= \det(\lambda - \hat{A}) \\ &= \lambda^4 - 4\alpha\lambda^2 - 16\beta\lambda + 16\gamma, \end{aligned} \quad (16.23)$$

where

$$\begin{aligned} \alpha &= c_1^2 + c_2^2 + c_3^2 + c_{12}^2 + c_{13}^2 + c_{23}^2 \\ \beta &= c_1 c_2 c_{12} + c_1 c_3 c_{13} + c_2 c_3 c_{23} + c_{12} c_{13} c_{23} \\ \gamma &= c_1^2 c_{23}^2 + c_2^2 c_{13}^2 + c_3^2 c_{12}^2 - 2c_1 c_2 c_{13} c_{23} - 2c_1 c_3 c_{12} c_{23} - 2c_2 c_3 c_{12} c_{13}. \end{aligned} \quad (16.24)$$

Simplifying, using results such as

$$c_1^2 + c_2^2 + c_{12}^2 = 1 + 2c_1 c_2 c_{12}, \quad (16.25)$$

we find

$$\beta = 1 + \frac{1}{2} \left(\cos \theta_1 + \cos \theta_2 + \cos \theta_3 + \cos(\theta_1 - \theta_2) + \cos(\theta_1 - \theta_3) + \cos(\theta_2 - \theta_3) \right) \quad (16.26)$$

and

$$\alpha = 2 + \beta, \quad \gamma = 1 - \beta. \quad (16.27)$$

The function $\beta(\boldsymbol{\theta})$ takes its minimum value of $\beta_{\min} = 0$ at $\boldsymbol{\theta} = \frac{\pi}{2}(1, 1, 0)$ (and at symmetry-related points in the Brillouin zone). The maximum occurs at the zone center $\boldsymbol{\theta} = 0$, where $\beta_{\max} = 4$.

The characteristic polynomial may be factored, using the results of eqn. 16.27. If we define $\lambda \equiv \varepsilon - 2$, then

$$\begin{aligned} P(\varepsilon - 2) &= \varepsilon^4 - 8\varepsilon^3 + 4(6 - \alpha)\varepsilon^2 + 16(2 + \beta - \alpha)\varepsilon + 16(1 - \alpha + 2\beta + \gamma) \\ &= \varepsilon^2 \left(\varepsilon^2 - 8\varepsilon + 4(4 - \beta) \right), \end{aligned} \quad (16.28)$$

and thus with $\lambda = \varepsilon - 2$ we have the four bands

$$\lambda_1 = -2, \quad \lambda_2 = -2, \quad \lambda_3 = 2 - 2\sqrt{\beta}, \quad \lambda_4 = 2 + 2\sqrt{\beta}. \quad (16.29)$$

Note that there are two flat bands at $\lambda_{1,2} = -2$. Note also that the largest eigenvalue is $\lambda_{4,\max} = 2 + 2\beta_{\max}^{1/2} = 6$, which is (correctly) the lattice coordination number. To make contact with some results of ref. 1, the adjacency matrix in eqn. 4 of ref. 1 is equivalent to $\hat{A} + 2$, hence the eigenvalues are our $\varepsilon_{1,2,3,4}$, which is to say $\varepsilon_{1,2} = 0$ and $\varepsilon_{3,4} = 4 \pm 2\sqrt{\beta}$. I presume that there is a typo and the eigenvalues $\nu_{1,2,3,4}$ in ref. 1 are for half the adjacency matrix.

For the electronic hopping Hamiltonian $\mathcal{H} = -t \sum_{\langle ij \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right)$ on the pyrochlore lattice, the energy eigenvalues are

$$E_1 = -2t - 2t\sqrt{\beta(\boldsymbol{\theta})}, \quad E_2 = -2t + 2t\sqrt{\beta(\boldsymbol{\theta})}, \quad E_{3,4} = +2t, \quad (16.30)$$

where $\beta(\boldsymbol{\theta}) \in [0, 4]$, as discussed above.

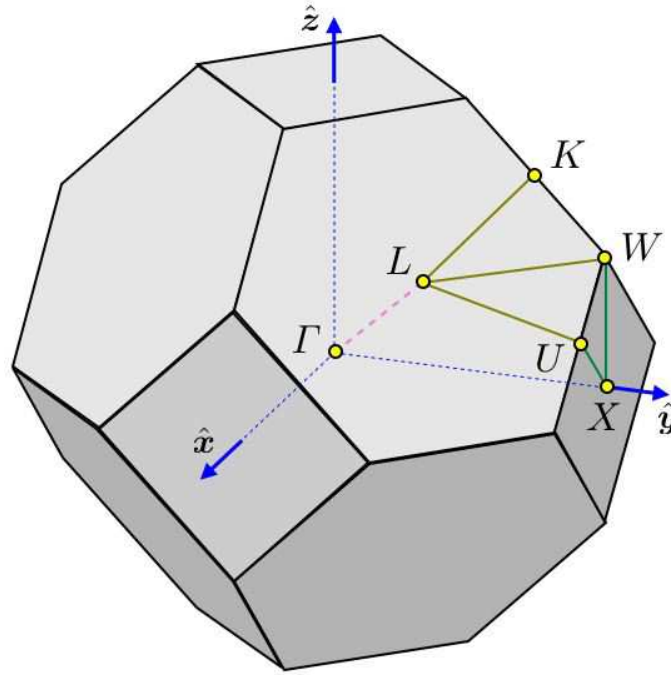


Figure 16.8: First Brillouin zone for an FCC structure, with high symmetry points labeled.

16.2.2 The FCC lattice Brillouin zone

Fig. 16.8 shows the first Brillouin zone for a (real space) FCC structure. Note that

$$\Gamma = (0, 0, 0) \quad (16.31)$$

$$L = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3) = \frac{\sqrt{2}\pi}{a} (1, 1, 1) \quad (16.32)$$

$$X = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_3) = \frac{\sqrt{2}\pi}{a} (0, 1, 0) . \quad (16.33)$$

Consider the point L' residing in the center of the hexagonal face adjacent to that containing L but with negative x coordinate. (This face is hidden in the figure.) One has

$$L' = \frac{1}{2}\mathbf{b}_1 = \frac{\sqrt{2}\pi}{a} (-1, 1, 1) . \quad (16.34)$$

To find W we note that it lies at the confluence of the two hexagonal faces containing L and L' , respectively, and the square face containing X . We may therefore write

$$\begin{aligned} W &= \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3) + r \cdot \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) + s \cdot \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_3) \\ W &= \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_3) + u \cdot \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) + v \cdot \frac{1}{2}(\mathbf{b}_2 + \mathbf{b}_3) \\ W &= \frac{1}{2}\mathbf{b}_1 + x \cdot \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2 + 2\mathbf{b}_3) + y \cdot \frac{1}{2}(\mathbf{b}_2 - \mathbf{b}_3) , \end{aligned} \quad (16.35)$$

where we must solve for (r, s, u, v, x, y) . What we have done here is to write the location of W as the location of each of the face centers plus an unknown vector lying in the plane of that face. Since the elementary reciprocal lattice vectors $\mathbf{b}_{1,2,3}$ are a linearly independent set, the coefficients of each elementary reciprocal lattice vector must independently sum to zero in the two equations which result from equating the first and second, and the second and third lines in eqn. 16.35. This yields six equations in our six unknowns, and solving for the unknowns we obtain

$$r = \frac{1}{2} \quad , \quad s = 0 \quad , \quad u = \frac{1}{2} \quad , \quad v = 0 \quad , \quad x = \frac{1}{2} \quad , \quad y = 0 \quad , \quad (16.36)$$

and therefore

$$W = \frac{3}{4}\mathbf{b}_1 + \frac{1}{4}\mathbf{b}_2 + \frac{1}{2}\mathbf{b}_3 = \frac{\sqrt{2}\pi}{a} \left(0, 1, \frac{1}{2}\right) . \quad (16.37)$$

Consider next the point W' lying on the other end of the edge containing U and K . We have

$$\begin{aligned} W' &= \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3) + r \cdot \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) + s \cdot \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_3) \\ W' &= \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) + u \cdot \frac{1}{2}(\mathbf{b}_2 + \mathbf{b}_3) + v \cdot \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_3) \\ W' &= \frac{1}{2}\mathbf{b}_1 + x \cdot \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2 + 2\mathbf{b}_3) + y \cdot \frac{1}{2}(\mathbf{b}_2 - \mathbf{b}_3) . \end{aligned} \quad (16.38)$$

Solving for the unknowns, we obtain

$$r = \frac{1}{2} \quad , \quad s = \frac{1}{2} \quad , \quad u = 0 \quad , \quad v = \frac{1}{2} \quad , \quad x = \frac{1}{2} \quad , \quad y = \frac{1}{2} \quad , \quad (16.39)$$

and therefore

$$W' = \frac{3}{4}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2 + \frac{1}{4}\mathbf{b}_3 = \frac{\sqrt{2}\pi}{a} \left(0, \frac{1}{2}, 1\right) . \quad (16.40)$$

Finally, consider the point W'' lying on the other end of the edge containing W and U . One then has

$$\begin{aligned} W &= \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3) + r \cdot \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) + s \cdot \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_3) \\ W &= \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_3) + u \cdot \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) + v \cdot \frac{1}{2}(\mathbf{b}_2 + \mathbf{b}_3) \\ W &= \frac{1}{2}\mathbf{b}_3 + x \cdot \frac{1}{2}(\mathbf{b}_1 - \mathbf{b}_2) + y \cdot \frac{1}{2}(\mathbf{b}_1 + 2\mathbf{b}_2 + \mathbf{b}_3) . \end{aligned} \quad (16.41)$$

Solving for the unknowns, we obtain

$$r = 0 \quad , \quad s = -\frac{1}{2} \quad , \quad u = 0 \quad , \quad v = \frac{1}{2} \quad , \quad x = \frac{1}{2} \quad , \quad y = \frac{1}{2} \quad , \quad (16.42)$$

and therefore

$$W'' = \frac{1}{2}\mathbf{b}_1 + \frac{1}{4}\mathbf{b}_2 + \frac{3}{4}\mathbf{b}_3 = \frac{\sqrt{2}\pi}{a} \left(\frac{1}{2}, 1, 0\right) . \quad (16.43)$$

Since K and U lie at the midpoints of WW' and WW'' respectively, we may now write

$$K = \frac{3}{4}\mathbf{b}_1 + \frac{3}{8}\mathbf{b}_2 + \frac{3}{8}\mathbf{b}_3 = \left(0, \frac{3}{4}, \frac{3}{4}\right) \quad (16.44)$$

$$U = \frac{5}{8}\mathbf{b}_1 + \frac{1}{4}\mathbf{b}_2 + \frac{5}{8}\mathbf{b}_3 = \left(\frac{1}{4}, 1, \frac{1}{4}\right) . \quad (16.45)$$

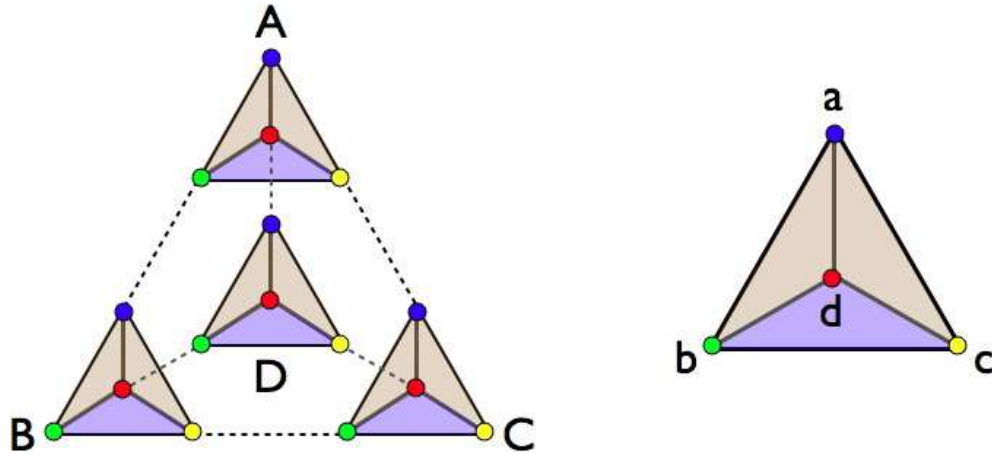


Figure 16.9: Supertetrahedron basis for the pyrochlore lattice.

16.3 Depleted Pyrochlores

16.3.1 Pyrochlore with 16 element basis

We change notation slightly. We define

$$\mathbf{a}_1 = \frac{1}{\sqrt{2}} a(0, 1, 1) \quad , \quad \mathbf{a}_2 = \frac{1}{\sqrt{2}} a(1, 0, 1) \quad , \quad \mathbf{a}_3 = \frac{1}{\sqrt{2}} a(1, 1, 0) . \quad (16.46)$$

Consider the 16 site basis for the pyrochlore lattice defined in Fig. 16.9, composed of a ‘supertetrahedron’ formed from four primary tetrahedra. The sites on each tetrahedron are labeled $\{a, b, c, d\}$ and the tetrahedra are labeled $\{A, B, C, D\}$. The origin is taken to be site Dd. The supertetrahedra form a simple cubic lattice with primary direct lattice vectors

$$\begin{aligned} \mathbf{c}_1 &= -\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 = \sqrt{2} a(1, 0, 0) \\ \mathbf{c}_2 &= +\mathbf{a}_1 - \mathbf{a}_2 + \mathbf{a}_3 = \sqrt{2} a(0, 1, 0) \\ \mathbf{c}_3 &= +\mathbf{a}_1 + \mathbf{a}_2 - \mathbf{a}_3 = \sqrt{2} a(0, 0, 1) . \end{aligned} \quad (16.47)$$

To see why the supertetrahedra fill all space with no missing tetrahedra, write the location of Dd on supertetrahedron (n_1, n_2, n_3) as

$$\begin{aligned} \mathbf{R}_{n_1, n_2, n_3} &= n_1 \mathbf{c}_1 + n_2 \mathbf{c}_2 + n_3 \mathbf{c}_3 \\ &= (-n_1 + n_2 + n_3) \mathbf{a}_1 + (n_1 - n_2 + n_3) \mathbf{a}_2 + (n_1 + n_2 - n_3) \mathbf{a}_3 \\ &\equiv \ell_1 \mathbf{a}_1 + \ell_2 \mathbf{a}_2 + \ell_3 \mathbf{a}_3 . \end{aligned} \quad (16.48)$$

Thus,

$$\ell_1 = -n_1 + n_2 + n_3 \quad , \quad \ell_2 = n_1 - n_2 + n_3 \quad , \quad \ell_3 = n_1 + n_2 - n_3 . \quad (16.49)$$

Note that $\ell_1 - \ell_2$, $\ell_2 - \ell_3$, and $\ell_3 - \ell_1$ are all even integers. $\mathbf{R}_{n_1, n_2, n_3}$ is the location of the Dd site in unit cell (n_1, n_2, n_3) . The location of the Ad site is then $\mathbf{R}_{n_1, n_2, n_3} + \mathbf{a}_1$. The location of the Bd site is $\mathbf{R}_{n_1, n_2, n_3} + \mathbf{a}_2$. The location of the Cd site is $\mathbf{R}_{n_1, n_2, n_3} + \mathbf{a}_3$. Thus, we have

$$\begin{aligned}
(\ell_1 - \ell_2, \ell_2 - \ell_3, \ell_3 - \ell_1) &= (\text{odd}, \text{odd}, \text{even}) \quad (\text{A}) \\
&= (\text{odd}, \text{even}, \text{odd}) \quad (\text{B}) \\
&= (\text{even}, \text{odd}, \text{odd}) \quad (\text{C}) \\
&= (\text{even}, \text{even}, \text{even}) \quad (\text{D}).
\end{aligned} \tag{16.50}$$

Since $(\ell_1 - \ell_2) + (\ell_2 - \ell_3) + (\ell_3 - \ell_1) = 0$, there number of odd differences must itself be even (*i.e.* 0 or 2). This exhausts all the possibilities for (ℓ_1, ℓ_2, ℓ_3) , so we have identified every tetrahedron.

The locations of the 16 sites in the $(0, 0, 0)$ supertetrahedron are then

$$\text{Aa} = \frac{3}{2}\mathbf{a}_1 \quad \text{Ab} = \mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 \quad \text{Ac} = \mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3 \quad \text{Ad} = \mathbf{a}_1 \tag{16.51}$$

$$\text{Ba} = \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_1 \quad \text{Bb} = \frac{3}{2}\mathbf{a}_2 \quad \text{Bc} = \mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3 \quad \text{Bd} = \mathbf{a}_2 \tag{16.52}$$

$$\text{Ca} = \mathbf{a}_3 + \frac{1}{2}\mathbf{a}_1 \quad \text{Cb} = \mathbf{a}_3 + \frac{1}{2}\mathbf{a}_2 \quad \text{Cc} = \frac{3}{2}\mathbf{a}_3 \quad \text{Cd} = \mathbf{a}_3 \tag{16.53}$$

$$\text{Da} = \frac{1}{2}\mathbf{a}_1 \quad \text{Db} = \frac{1}{2}\mathbf{a}_2 \quad \text{Dc} = \frac{1}{2}\mathbf{a}_3 \quad \text{Dd} = 0. \tag{16.54}$$

The Fourier transform of the adjacency matrix is given by

$$M(\boldsymbol{\theta}) = \begin{pmatrix}
& \text{Aa} & \text{Ab} & \text{Ac} & \text{Ad} & \text{Ba} & \text{Bb} & \text{Bc} & \text{Bd} & \text{Ca} & \text{Cb} & \text{Cc} & \text{Cd} & \text{Da} & \text{Db} & \text{Dc} & \text{Dd} \\
\text{Aa} & 0 & 1 & 1 & 1 & 0 & \bar{z}_1 z_2 & 0 & 0 & 0 & 0 & \bar{z}_1 z_3 & 0 & 0 & 0 & 0 & z_2 z_3 \\
\text{Ab} & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & z_3 & 0 & 0 & z_3 & 0 \\
\text{Ac} & 1 & 1 & 0 & 1 & 0 & 0 & 0 & z_2 & 1 & 0 & 0 & 0 & 0 & z_2 & 0 & 0 \\
\text{Ad} & 1 & 1 & 1 & 0 & 0 & 0 & \bar{z}_1 & 0 & 0 & \bar{z}_1 & 0 & 0 & 1 & 0 & 0 & 0 \\
\text{Ba} & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & z_3 & 0 & 0 & z_3 & 0 \\
\text{Bb} & z_1 \bar{z}_2 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & \bar{z}_2 z_3 & 0 & 0 & 0 & 0 & z_1 z_3 \\
\text{Bc} & 0 & 0 & 0 & z_1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & z_1 & 0 & 0 & 0 \\
\text{Bd} & 0 & 0 & \bar{z}_2 & 0 & 1 & 1 & 1 & 0 & \bar{z}_2 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
\text{Ca} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & z_2 & 0 & 1 & 1 & 1 & 0 & z_2 & 0 & 0 \\
\text{Cb} & 0 & 0 & 0 & z_1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & z_1 & 0 & 0 & 0 \\
\text{Cc} & z_1 \bar{z}_3 & 0 & 0 & 0 & 0 & z_2 \bar{z}_3 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & z_1 z_2 \\
\text{Cd} & 0 & \bar{z}_3 & 0 & 0 & \bar{z}_3 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\
\text{Da} & 0 & 0 & 0 & 1 & 0 & 0 & \bar{z}_1 & 0 & 0 & \bar{z}_1 & 0 & 0 & 0 & 1 & 1 & 1 \\
\text{Db} & 0 & 0 & \bar{z}_2 & 0 & 0 & 0 & 0 & 1 & \bar{z}_2 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\
\text{Dc} & 0 & \bar{z}_3 & 0 & 0 & \bar{z}_3 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \\
\text{Dd} & \bar{z}_2 \bar{z}_3 & 0 & 0 & 0 & 0 & \bar{z}_1 \bar{z}_3 & 0 & 0 & 0 & 0 & \bar{z}_1 \bar{z}_2 & 0 & 1 & 1 & 1 & 0
\end{pmatrix}$$

where $z_j = e^{i\theta_j}$ with $j \in \{1, 2, 3\}$. The way to read this matrix is as follows. There are six nonzero entries in each row and in each column, corresponding to coordination number six.

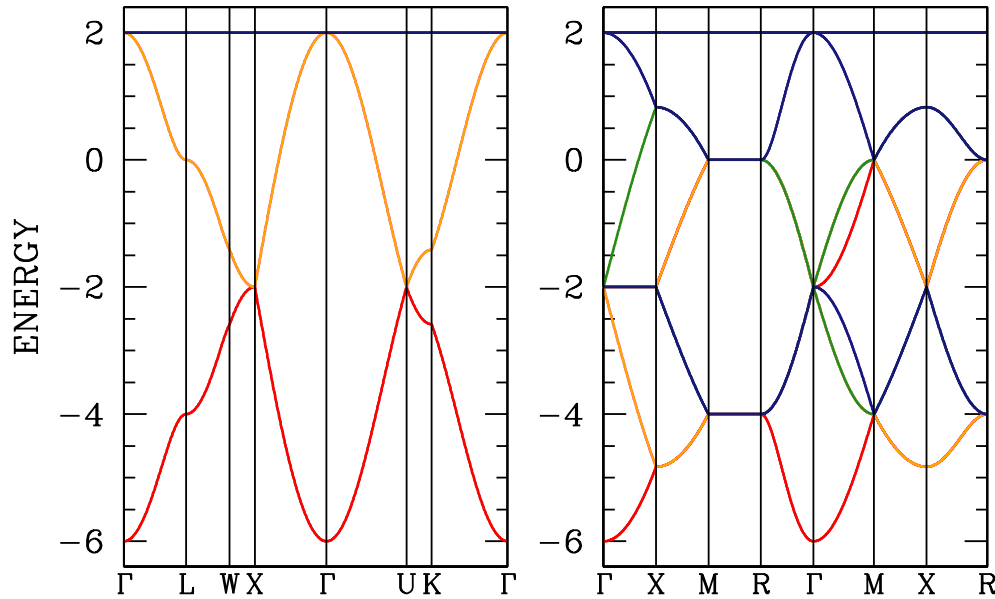


Figure 16.10: Comparison of pyrochlore band structures computed in 4-element FCC basis (left) and 16-element SC basis (right).

The rows correspond to sites Aa (1) through Dd (16). Reading along the first row, we see that Aa has neighbors Ab, Ac, and Ad in the unit cell $(0, 0, 0)$, as well as a neighbor Bb in unit cell $\mathbf{c}_2 - \mathbf{c}_1$ (from $M_{16} = \bar{z}_1 z_2$), a neighbor Cc in unit cell $\mathbf{c}_3 - \mathbf{c}_1$, and a neighbor Dd in unit cell $\mathbf{c}_2 + \mathbf{c}_3$. The Hamiltonian is then $H(\boldsymbol{\theta}) = -t M(\boldsymbol{\theta})$.

The high-symmetry points in the cubic lattice Brillouin zone are as follows:

$$\begin{aligned}
 \Gamma &: (\theta_1, \theta_2, \theta_3) = (0, 0, 0) && \text{(zone center)} \\
 X &: (\theta_1, \theta_2, \theta_3) = (\pi, 0, 0) && \text{(face center)} \\
 M &: (\theta_1, \theta_2, \theta_3) = (\pi, \pi, 0) && \text{(edge center)} \\
 R &: (\theta_1, \theta_2, \theta_3) = (\pi, \pi, \pi) && \text{(zone corner)}.
 \end{aligned} \tag{16.55}$$

In Fig. 16.10, we plot the dispersion for the tight binding Hamiltonian on the pyrochlore lattice with $t = 1$ using both the 4-element FCC basis as well as the 16-element SC basis.

For the Kondo Hamiltonian with fixed local moments, we write

$$H(\boldsymbol{\theta}) = -t \sum_{a,b=1}^{16} \sum_{\mu=1}^2 M_{ab}(\boldsymbol{\theta}) c_{a,\mu}^\dagger(\boldsymbol{\theta}) c_{b,\mu}(\boldsymbol{\theta}) - J \sum_{a=1}^{16} \sum_{\mu,\nu=1}^2 \hat{\mathbf{n}}_a \cdot c_{a,\mu}^\dagger(\boldsymbol{\theta}) \boldsymbol{\sigma}_{\mu\nu} c_{a,\nu}(\boldsymbol{\theta}), \tag{16.56}$$

where J is the Kondo coupling and $\hat{\mathbf{n}}_a$ is the direction of the local moment, with all local moments assumed to be of unit magnitude. At each $\boldsymbol{\theta}$ point in the Brillouin zone, the Hamiltonian is a 32×32 matrix.

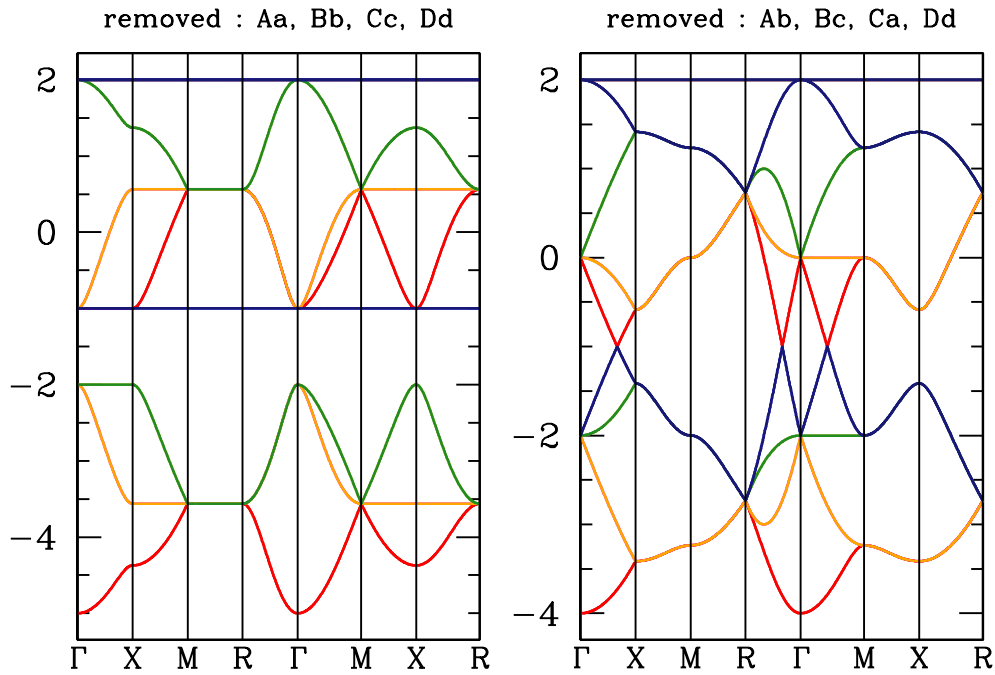


Figure 16.11: Comparison of depleted pyrochlore band structures ($t = 1$, $J = 0$). Left panel: sites Aa, Bb, Cc, Dd removed. Right panel: sites Ab, Bc, Ca, Dd removed.

16.3.2 Depleted pyrochlore

To deplete the pyrochlore, we knock out rows and columns of M . Equivalently, we can add an infinite on-site energy to the diagonal elements $H_{aa}(\theta)$. For the Kondo Hamiltonian, we add the infinite on-site energy to $H_{a\uparrow, a\uparrow}(\theta)$ and $H_{a\downarrow, a\downarrow}(\theta)$. In Fig. 16.11 we plot the band structures for two depleted pyrochlore structures, one in which sites Aa, Bb, Cc, and Dd have been removed (I), and another in which sites Ab, Bc, Ca, and Dd have been removed (II). The resulting structures may not have the full cubic lattice symmetry.

Eliminating the necessary rows and columns from $M(\theta)$, we arrive at the adjacency matrices

for the two depleted structures (I) and (II). We find for (I),

$$M^{(I)}(\boldsymbol{\theta}) = \begin{pmatrix} & \text{Ab} & \text{Ac} & \text{Ad} & \text{Ba} & \text{Bc} & \text{Bd} & \text{Ca} & \text{Cb} & \text{Cd} & \text{Da} & \text{Db} & \text{Dc} \\ \text{Ab} & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & z_3 & 0 & 0 & z_3 \\ \text{Ac} & 1 & 0 & 1 & 0 & 0 & z_2 & 1 & 0 & 0 & 0 & z_2 & 0 \\ \text{Ad} & 1 & 1 & 0 & 0 & \bar{z}_1 & 0 & 0 & \bar{z}_1 & 0 & 1 & 0 & 0 \\ \text{Ba} & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & z_3 & 0 & 0 & z_3 \\ \text{Bc} & 0 & 0 & z_1 & 1 & 0 & 1 & 0 & 1 & 0 & z_1 & 0 & 0 \\ \text{Bd} & 0 & \bar{z}_2 & 0 & 1 & 1 & 0 & \bar{z}_2 & 0 & 0 & 0 & 1 & 0 \\ \text{Ca} & 0 & 1 & 0 & 0 & 0 & z_2 & 0 & 1 & 1 & 0 & z_2 & 0 \\ \text{Cb} & 0 & 0 & z_1 & 0 & 1 & 0 & 1 & 0 & 1 & z_1 & 0 & 0 \\ \text{Cd} & \bar{z}_3 & 0 & 0 & \bar{z}_3 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ \text{Da} & 0 & 0 & 1 & 0 & \bar{z}_1 & 0 & 0 & \bar{z}_1 & 0 & 0 & 1 & 1 \\ \text{Db} & 0 & \bar{z}_2 & 0 & 0 & 0 & 1 & \bar{z}_2 & 0 & 0 & 1 & 0 & 1 \\ \text{Dc} & \bar{z}_3 & 0 & 0 & \bar{z}_3 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix}.$$

This corresponds to a five-fold coordinated structure, since there are five nonzero elements in each row and each column. For the (II) structure, we have

$$M^{(II)}(\boldsymbol{\theta}) = \begin{pmatrix} & \text{Aa} & \text{Ac} & \text{Ad} & \text{Ba} & \text{Bb} & \text{Bd} & \text{Cb} & \text{Cc} & \text{Cd} & \text{Da} & \text{Db} & \text{Dc} \\ \text{Aa} & 0 & 1 & 1 & 0 & \bar{z}_1 z_2 & 0 & 0 & \bar{z}_1 z_3 & 0 & 0 & 0 & 0 \\ \text{Ac} & 1 & 0 & 1 & 0 & 0 & z_2 & 0 & 0 & 0 & 0 & z_2 & 0 \\ \text{Ad} & 1 & 1 & 0 & 0 & 0 & 0 & \bar{z}_1 & 0 & 0 & 1 & 0 & 0 \\ \text{Ba} & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & z_3 & 0 & 0 & z_3 \\ \text{Bb} & z_1 \bar{z}_2 & 0 & 0 & 1 & 0 & 1 & 0 & \bar{z}_2 z_3 & 0 & 0 & 0 & 0 \\ \text{Bd} & 0 & \bar{z}_2 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ \text{Cb} & 0 & 0 & z_1 & 0 & 0 & 0 & 0 & 1 & 1 & z_1 & 0 & 0 \\ \text{Cc} & z_1 \bar{z}_3 & 0 & 0 & 0 & z_2 \bar{z}_3 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ \text{Cd} & 0 & 0 & 0 & \bar{z}_3 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ \text{Da} & 0 & 0 & 1 & 0 & 0 & 0 & \bar{z}_1 & 0 & 0 & 0 & 1 & 1 \\ \text{Db} & 0 & \bar{z}_2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ \text{Dc} & 0 & 0 & 0 & \bar{z}_3 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix},$$

corresponding to a four-fold coordinated structure, known as the hyperkagome lattice.

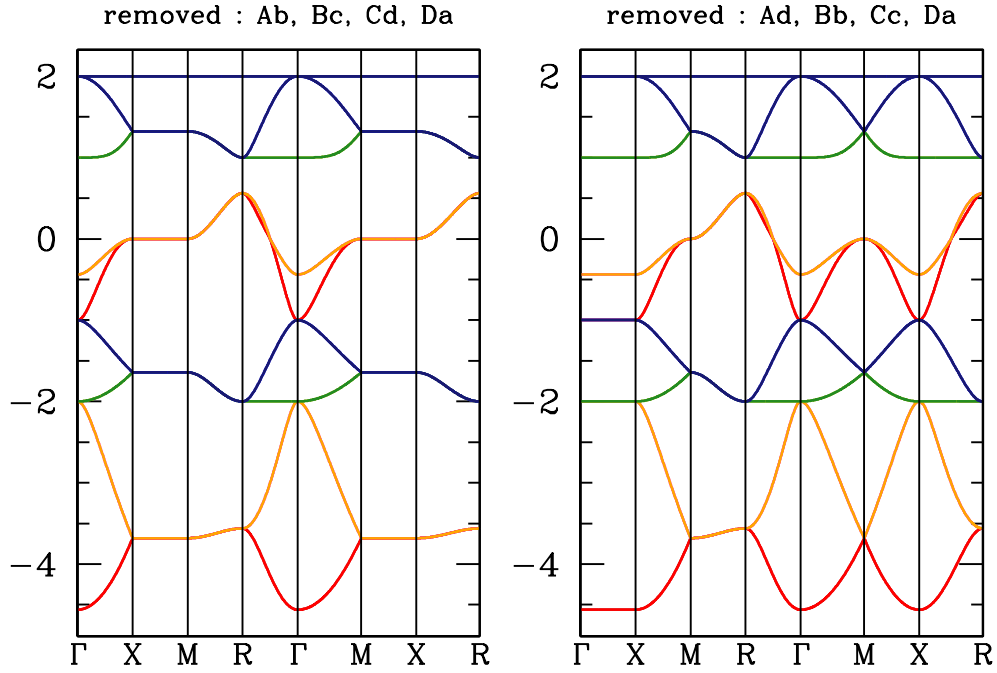


Figure 16.12: Comparison of two additional depleted pyrochlore band structures III and IV ($t = 1, J = 0$).

The energy bands for two additional structures are shown in Fig. 16.12. We find

$$M^{(\text{III})}(\theta) = \begin{pmatrix} & \text{Aa} & \text{Ac} & \text{Ad} & \text{Ba} & \text{Bb} & \text{Bd} & \text{Ca} & \text{Cb} & \text{Cc} & \text{Db} & \text{Dc} & \text{Dd} \\ \text{Aa} & 0 & 1 & 1 & 0 & \bar{z}_1 z_2 & 0 & 0 & 0 & \bar{z}_1 z_3 & 0 & 0 & z_2 z_3 \\ \text{Ac} & 1 & 0 & 1 & 0 & 0 & z_2 & 1 & 0 & 0 & z_2 & 0 & 0 \\ \text{Ad} & 1 & 1 & 0 & 0 & 0 & 0 & 0 & \bar{z}_1 & 0 & 0 & 0 & 0 \\ \text{Ba} & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & z_3 & 0 \\ \text{Bb} & z_1 \bar{z}_2 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & \bar{z}_2 z_3 & 0 & 0 & z_1 z_3 \\ \text{Bd} & 0 & \bar{z}_2 & 0 & 1 & 1 & 0 & \bar{z}_2 & 0 & 0 & 1 & 0 & 0 \\ \text{Ca} & 0 & 1 & 0 & 0 & 0 & z_2 & 0 & 1 & 1 & z_2 & 0 & 0 \\ \text{Cb} & 0 & 0 & z_1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ \text{Cc} & z_1 \bar{z}_3 & 0 & 0 & 0 & z_2 \bar{z}_3 & 0 & 1 & 1 & 0 & 0 & 0 & z_1 z_2 \\ \text{Db} & 0 & \bar{z}_2 & 0 & 0 & 0 & 1 & \bar{z}_2 & 0 & 0 & 0 & 1 & 1 \\ \text{Dc} & 0 & 0 & 0 & \bar{z}_3 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ \text{Dd} & \bar{z}_2 \bar{z}_3 & 0 & 0 & 0 & \bar{z}_1 \bar{z}_3 & 0 & 0 & 0 & \bar{z}_1 \bar{z}_2 & 1 & 1 & 0 \end{pmatrix}$$

In this structure, nine of the 12 sites are 5-fold coordinated, and the remaining three are 3-fold

coordinated. What seems to be an equivalent structure is (IV):

$$M^{(\text{IV})}(\boldsymbol{\theta}) = \begin{pmatrix} & \text{Aa} & \text{Ab} & \text{Ac} & \text{Ba} & \text{Bc} & \text{Bd} & \text{Ca} & \text{Cb} & \text{Cd} & \text{Db} & \text{Dc} & \text{Dd} \\ \text{Aa} & 0 & 1 & 1 & 0 & \bar{z}_1 z_2 & 0 & 0 & 0 & 0 & 0 & 0 & z_2 z_3 \\ \text{Ab} & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & z_3 & 0 & z_3 & 0 \\ \text{Ac} & 1 & 0 & 1 & 0 & 0 & z_2 & 1 & 0 & 0 & z_2 & 0 & 0 \\ \text{Ba} & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & z_3 & 0 & z_3 & 0 \\ \text{Bc} & 0 & 0 & z_1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ \text{Bd} & 0 & \bar{z}_2 & 0 & 1 & 1 & 0 & \bar{z}_2 & 0 & 0 & 1 & 0 & 0 \\ \text{Ca} & 0 & 1 & 0 & 0 & 0 & z_2 & 0 & 1 & 1 & z_2 & 0 & 0 \\ \text{Cb} & 0 & 0 & z_1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ \text{Cd} & 0 & 0 & 0 & \bar{z}_3 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ \text{Db} & 0 & \bar{z}_2 & 0 & 0 & 0 & 1 & \bar{z}_2 & 0 & 0 & 0 & 1 & 1 \\ \text{Dc} & 0 & 0 & 0 & \bar{z}_3 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \\ \text{Dd} & \bar{z}_2 \bar{z}_3 & 0 & 0 & 0 & \bar{z}_1 \bar{z}_3 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

16.4 References

- [1] S. Isakov, K. Gregor, R. Moessner, and S. L. Sondhi, *Phys. Rev. Lett.* **93**, 106702 (2004).