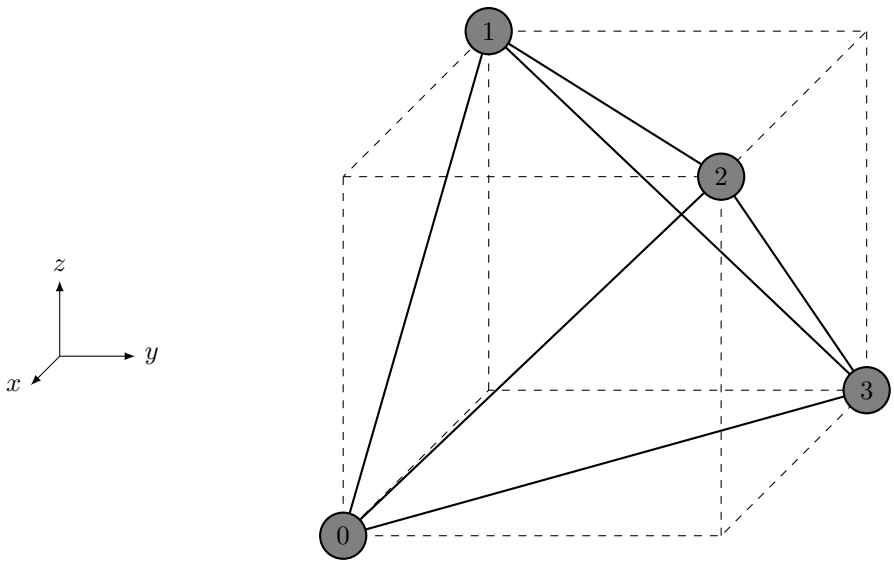
Symmetries of the Tetrahedron



The idea is to use the symmetries of the regular tetrahedron to aid in the diagonalisation of H.[1] This is S_4, the group of all permutation of four objects, from which the largest two *abelian* subgroups are K_4, the Kelin four group, and C_4, the cyclic group of order 4.

The elements of the former are π rotations of the tetrahedron about the three coordinate axes. Performing these operations one obtains the representation

$$K_4: \qquad R_x = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \qquad R_y = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad R_z = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

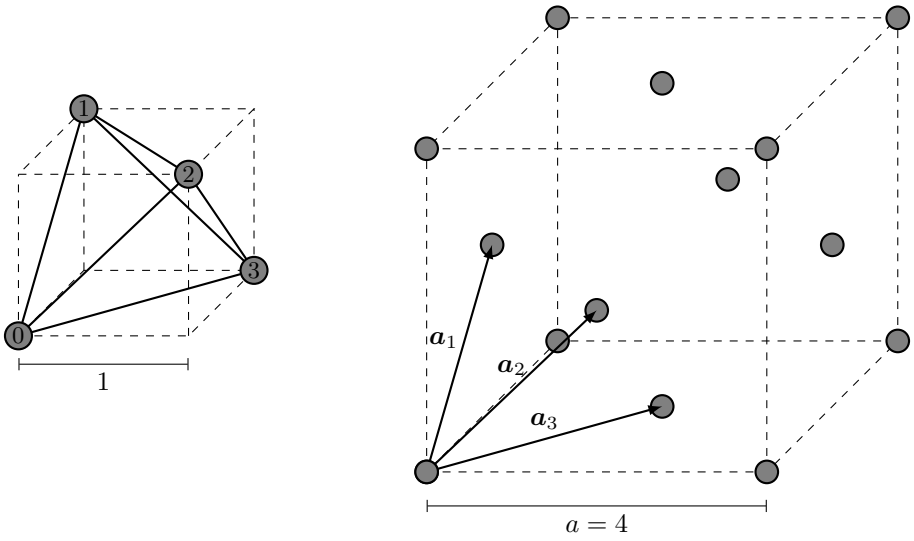
$$K_4: \qquad \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \end{bmatrix} \qquad \begin{bmatrix} -1 \\ 1 \\ 1 \\ -1 \end{bmatrix}$$

$$\begin{array}{cccc} R_x = +1 & R_x = -1 & R_x = +1 & R_x = -1 \\ R_y = +1 & R_y = +1 & R_y = -1 & R_y = -1 \\ R_z = R_x R_y = +1 & R_z = -1 & R_z = -1 & R_z = +1 \end{array}$$

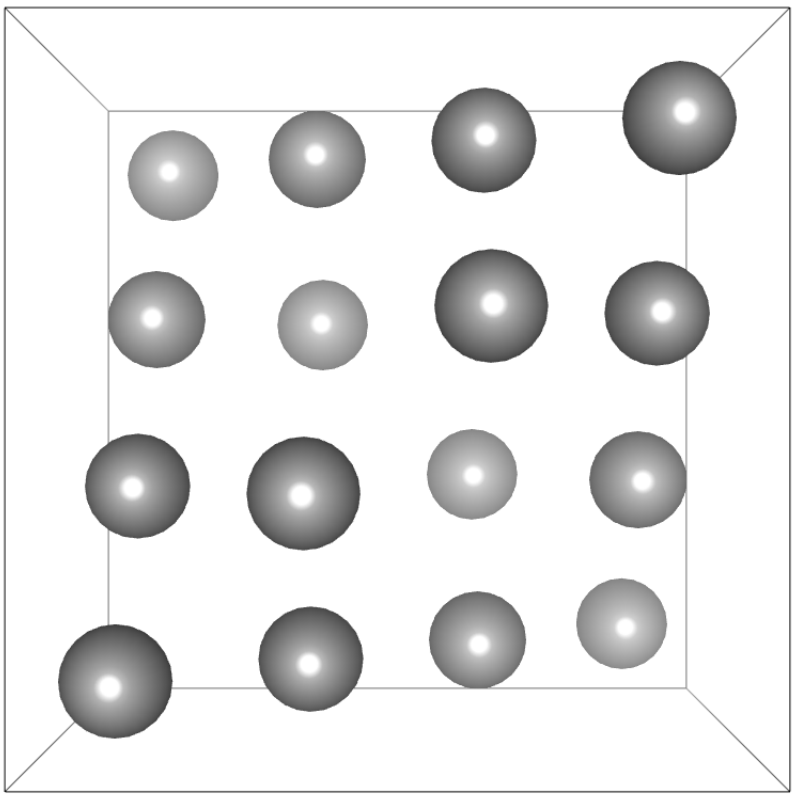
[1] Recall that a symmetry of the Hamiltonian H is a unitary transformation T_1 which commutes with H, implying that T_1 and H may be simultaneously diagonalised. It follows that if one diagonalises T_1, then H will also be diagonal or at least reduced to block diagonal form. In the latter case it is appropriate to introduce additional commuting symmetry T_2, T_3,... in order to nail down a unique common eigenbasis.

Pyrochlore

To generate pyrochlore, place a tetrahedral arrangement of sites at each point of an face-centred-cubic (fcc) lattice (here $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ are primitive lattice vectors):

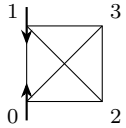


Members of the pyrochlore mineral group $A_2B_2O_6O$' provide real-world realisations of the pyrochlore structure. Here *both* A and B atoms (typically rare-earth or transition metals) are in tetrahedral arrangements, forming two interpentrating arrays of corner-sharing tetrahedra. An example is $Ca_2Nb_2O_6F$; below is a view of the Ca atoms in a single unit cell.

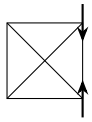


Opposite Spins

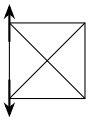
Each spin is free to occupy any of the four sites independently of the other, giving $4^2 = 16$ states, 4 involving double occupation. The rotations in K_4 were used to organise the states below (the states in each row being related by a rotation).



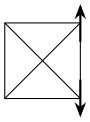
$|1\rangle = c^\dagger_{0\uparrow} c^\dagger_{1\downarrow} |0\rangle$



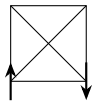
$|2\rangle = c^\dagger_{2\uparrow} c^\dagger_{3\downarrow} |0\rangle$



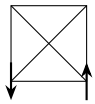
$|3\rangle = c^\dagger_{1\uparrow} c^\dagger_{0\downarrow} |0\rangle$



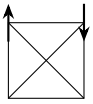
$|4\rangle = c^\dagger_{3\uparrow} c^\dagger_{2\downarrow} |0\rangle$



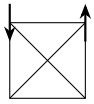
$|5\rangle = c^\dagger_{0\uparrow} c^\dagger_{2\downarrow} |0\rangle$



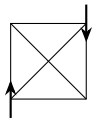
$|6\rangle = c^\dagger_{2\uparrow} c^\dagger_{0\downarrow} |0\rangle$



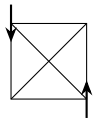
$|7\rangle = c^\dagger_{1\uparrow} c^\dagger_{3\downarrow} |0\rangle$



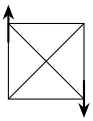
$|8\rangle = c^\dagger_{3\uparrow} c^\dagger_{1\downarrow} |0\rangle$



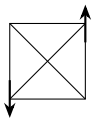
$|9\rangle = c^\dagger_{0\uparrow} c^\dagger_{3\downarrow} |0\rangle$



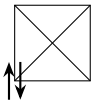
$|10\rangle = c^\dagger_{2\uparrow} c^\dagger_{1\downarrow} |0\rangle$



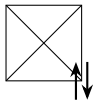
$|11\rangle = c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} |0\rangle$



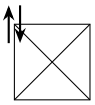
$|12\rangle = c^\dagger_{3\uparrow} c^\dagger_{0\downarrow} |0\rangle$



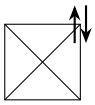
$|13\rangle = c^\dagger_{0\uparrow} c^\dagger_{0\downarrow} |0\rangle$



$|14\rangle = c^\dagger_{2\uparrow} c^\dagger_{2\downarrow} |0\rangle$



$|15\rangle = c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} |0\rangle$



$|16\rangle = c^\dagger_{3\uparrow} c^\dagger_{3\downarrow} |0\rangle$

Writing down H is a matter of determining which states are related by a single hop (movement of one spin to an adjacent site). For instance, $\langle 5|H|1\rangle = -t$ while $\langle 2|H|1\rangle = 0$. Remembering that $|13\rangle - |16\rangle$ also involve a U term, one obtains

$$H = \left[\begin{array}{cccc:cccc:cccc:cccc}
0 & 0 & 0 & 0 & -t & 0 & 0 & -t & -t & -t & 0 & 0 & -t & 0 & -t & 0 \\
0 & 0 & 0 & 0 & 0 & -t & -t & 0 & -t & -t & 0 & 0 & 0 & -t & 0 & -t \\
0 & 0 & 0 & 0 & 0 & -t & -t & 0 & 0 & 0 & -t & -t & -t & 0 & -t & 0 \\
0 & 0 & 0 & 0 & -t & 0 & 0 & -t & 0 & 0 & -t & -t & 0 & -t & 0 & -t \\
\hdashline
-t & 0 & 0 & -t & 0 & 0 & 0 & 0 & -t & 0 & -t & 0 & -t & -t & 0 & 0 \\
0 & -t & -t & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & -t & -t & -t & 0 & 0 \\
0 & -t & -t & 0 & 0 & 0 & 0 & 0 & -t & 0 & -t & 0 & 0 & 0 & -t & -t \\
-t & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & -t & 0 & -t & 0 & 0 & -t & -t \\
\hdashline
-t & -t & 0 & 0 & -t & 0 & -t & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & -t \\
-t & -t & 0 & 0 & 0 & -t & 0 & -t & 0 & 0 & 0 & 0 & 0 & -t & -t & 0 \\
0 & 0 & -t & -t & -t & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & -t & -t & 0 \\
0 & 0 & -t & -t & 0 & -t & 0 & -t & 0 & 0 & 0 & 0 & -t & 0 & 0 & -t \\
\hdashline
-t & 0 & -t & 0 & -t & -t & 0 & 0 & -t & 0 & 0 & -t & U & 0 & 0 & 0 \\
0 & -t & 0 & -t & -t & -t & 0 & 0 & 0 & -t & -t & 0 & 0 & U & 0 & 0 \\
-t & 0 & -t & 0 & 0 & 0 & -t & -t & 0 & -t & -t & 0 & 0 & 0 & U & 0 \\
0 & -t & 0 & -t & 0 & 0 & -t & -t & -t & 0 & 0 & -t & 0 & 0 & 0 & U
\end{array}\right]$$

The K_4 matrices can then be identified

$$H = \left[\begin{array}{c|c|c|c} O_{4\times4} & -t(1+R_z) & -t(1+R_y) & -t(1+R_x) \\ \hline -t(1+R_z) & O_{4\times4} & -t(1+R_x) & -t(1+R_y) \\ \hline -t(1+R_y) & -t(1+R_x) & O_{4\times4} & -t(1+R_z) \\ \hline -t(1+R_x) & -t(1+R_y) & -t(1+R_z) & U \end{array}\right]$$

Given this form, it is natural to look to an 16-eigenvector based on the vectors of the K_4 basis. For example, writing $\boldsymbol{v} = [1,1,1,1]^T$, we look for a solution of the form $[a\boldsymbol{v}, b\boldsymbol{v}, c\boldsymbol{v}, d\boldsymbol{v}]^T$ where a, b, c, d are unknown constants. Since $\boldsymbol{v}$ is an eigenvector or each 4x4 block, we have the effective 4-dimensional eigenvalue problem $A\boldsymbol{a} = (-E/2t)\boldsymbol{a}$ with

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & -U/2t \end{pmatrix}, \quad \boldsymbol{a} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

The characteristic equation is

$$\chi(\epsilon) = -48t^4 + 64t^3\epsilon - 24t^2\epsilon^2 + \epsilon^4 - U(\epsilon+4t)(\epsilon-2t)^2 = P_4 + UP_3$$

When $U = \infty$, P_3 gives the least root $-4t$. For $U \gg t$ finite, this is subject to a small correction:

$$0 = P_4 + UP_3 \to \epsilon = -4t + \left.\frac{P_4}{U(\epsilon-2t)^2}\right|_{\epsilon=-4t} = -4t - \frac{12t^2}{U}$$

which provides the ground state energy and its $1/U$ correction (the other three K_4 vectors yield a lowest energy $-2t + O(1/U)$ – Exercise). To determine the corresponding eigenvector when $U \to \infty$, note that to satisfy the eigenvalue equation in this limit the final entry of $\boldsymbol{a}$ must vanish. This means we can 'knock out' the final row and column of A and consider

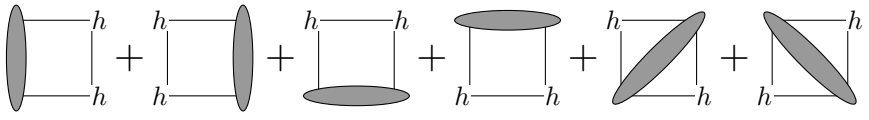
$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \widetilde{\boldsymbol{a}} = (-E/2t)\widetilde{\boldsymbol{a}} = 2\widetilde{\boldsymbol{a}} \to \widetilde{\boldsymbol{a}} = (1,1,1)^T \to \boldsymbol{a} = (1,1,1,0)^T$$

or

$$[1,1,1,1,1,1,1,1,1,1,1,1,0,0,0,0]^T$$

in the original basis.

Unsurprisingly, this is an equally weighted superposition of all states with single occupation only. Writing out the state in full using the operators on the previous page, one finds that the corresponding picture is



where each ellipse indicates a singlet between neighbouring sites and h a vacancy (e.g. the leftmost schematic represents $[c^\dagger_{0\uparrow}c^\dagger_{1\downarrow} - c^\dagger_{0\downarrow}c^\dagger_{1\uparrow}]\,|0\rangle$).