Spin Correlation Functions on Pyrochlore Lattice

Chen Wei
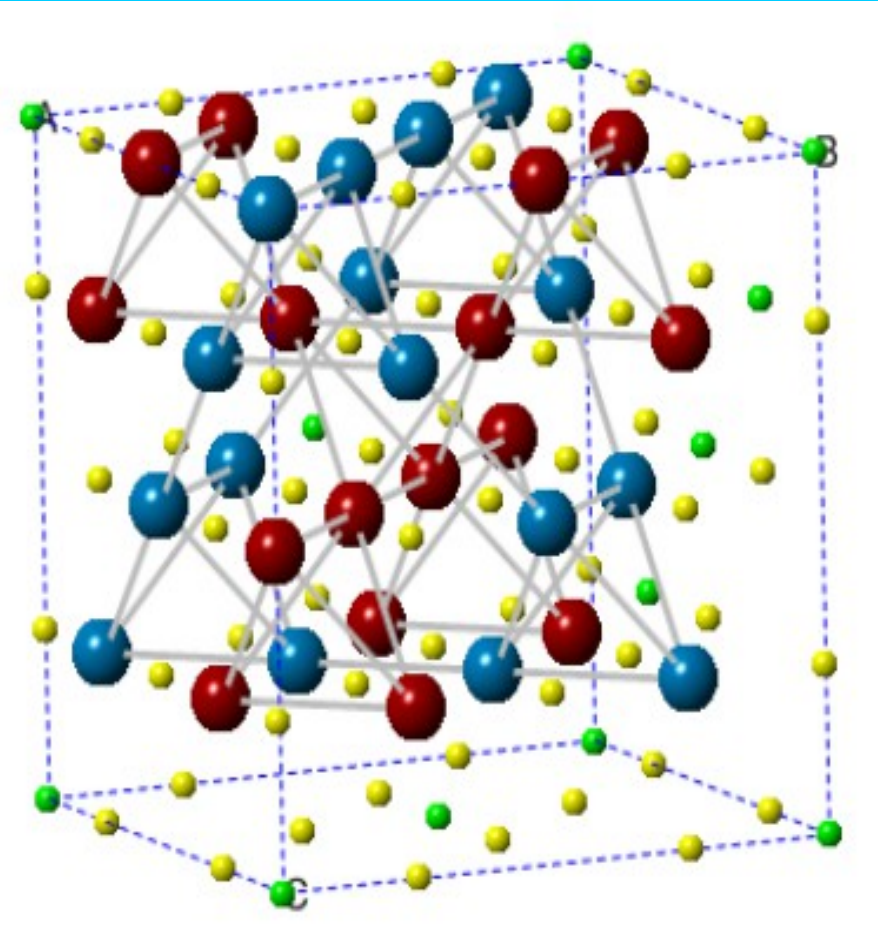
Supervisor: Dr. Stephanie H. Curnoe

Abstract: Pyrochlores have the chemical formula $A_2B_2O_7$ with A, B or both magnetic. It has corner-sharing tetrahedra in the structure. Here, I will focus on $Tb_2Ti_2O_7$, and use perturbation theory to find the spin correlation function.

Introduction: $Tb_2Ti_2O_7$ structure has space group No.227, the detail is listed In table 1.1.

Table 1.1: Space Group of $Tb_2Ti_2O_7$

Ions	Site	Coordinate Position
Terbium	16d	(0.5, 0.5, 0.5)
Titanium	16c	(0, 0, 0)
Oxygen	8b	(0.375, 0.375, 0.375)
Oxygen	48f	$(x, 0.125, 0.125)$

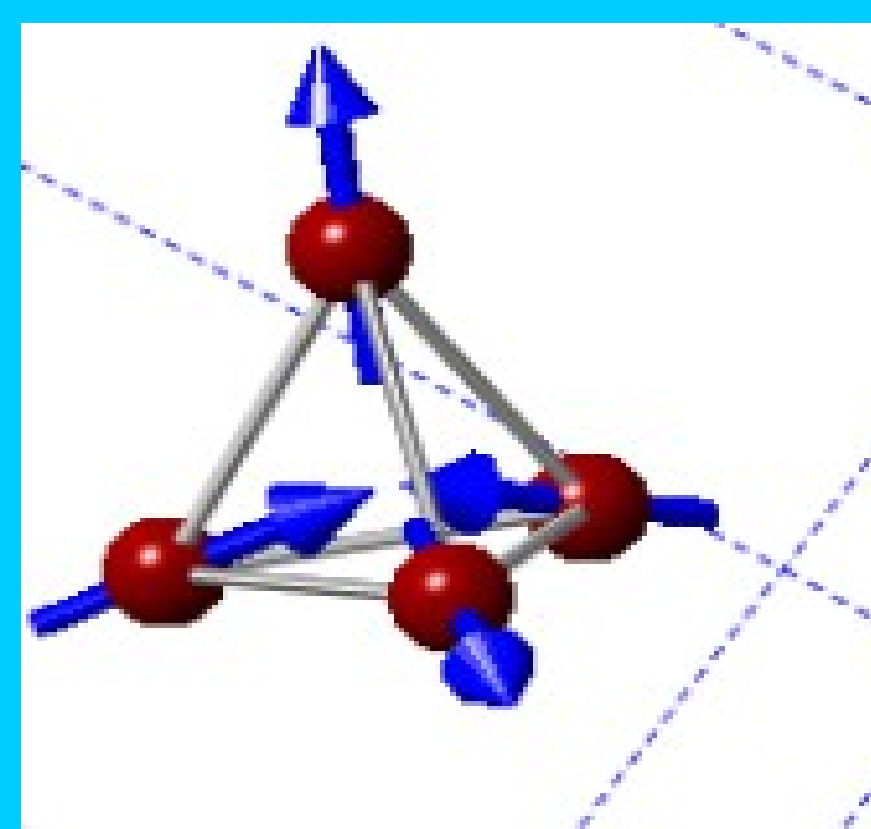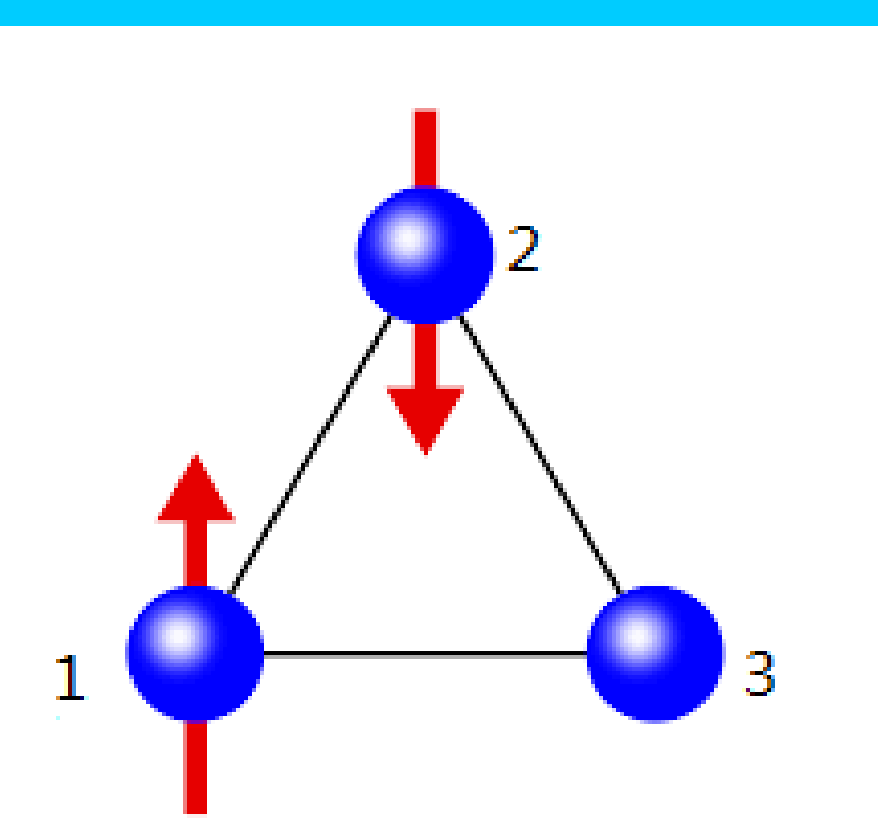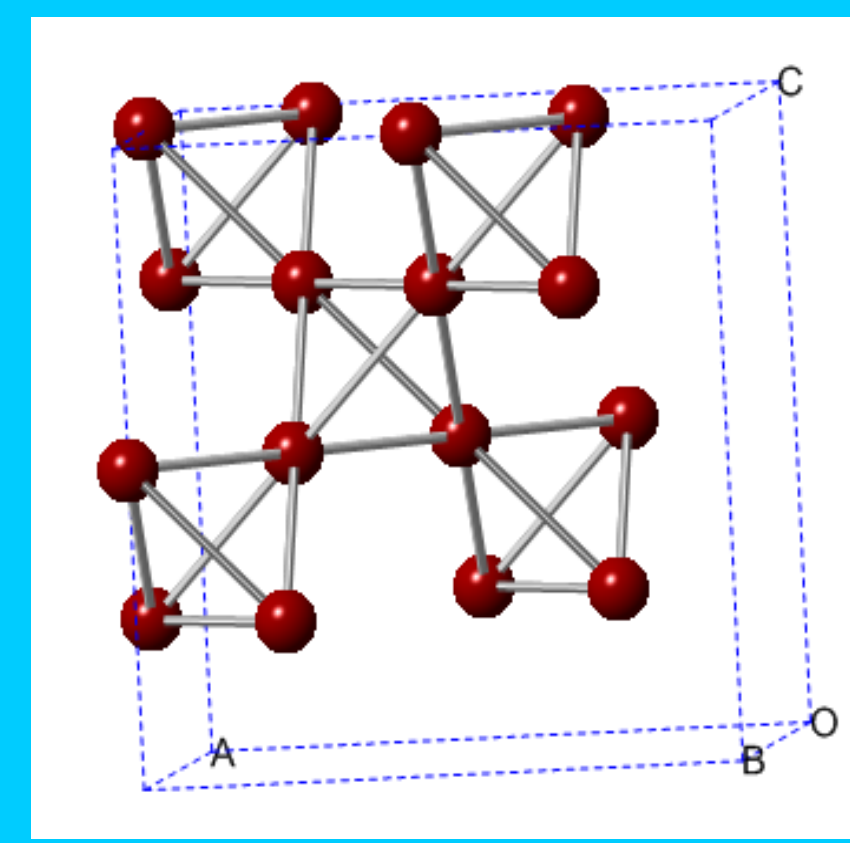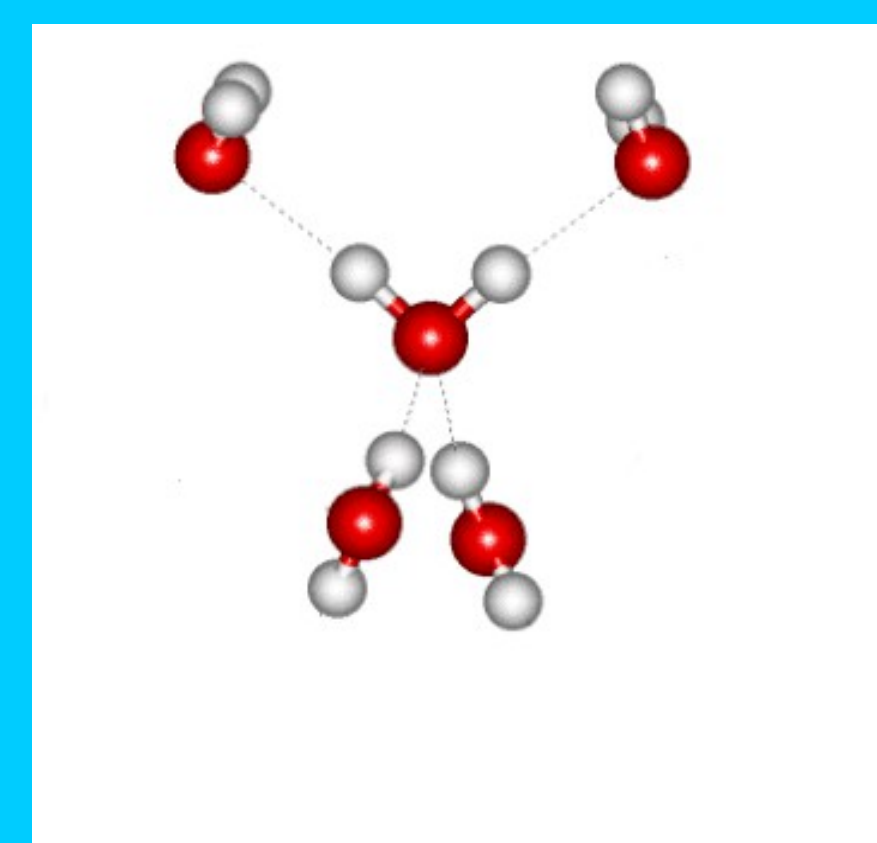**Why are we interested in $Tb_2Ti_2O_7$?** $Tb_2Ti_2O_7$ does not show any magnetic long-range order down to 50 mK and remains dynamic with short range correlations. Moreover, $Tb_2Ti_2O_7$ is a quantum spin ice and it is an example of geometric frustration.

Geometric Frustration:
Geometric frustration indicate the phenomenon that the system cannot minimize its total classical energy by minimizing the interaction energy between each pair of interacting degrees of freedom pair by pair due to its geometric structure of the lattice. One structure involved geometric frustration is crystal ice, and another example is spin ice.

Crystal Ice and Spin Ice: In 1935, Linus Pauling stated the ice rule for crystal ice which states that in crystal ice for each oxygen atom, there are two hydrogen close to it and two away from it. Therefore, crystal ice has residue entropy even at zero termperature. Spin ice material have the similar structure as crystal ice, in spin ice material, there are two ions with spin point outwards analogical to the away hydrogen atoms and two ions with spin point inwards analogical to the close hydrogen atoms.

Pauling's Argument in Spin Ice: Assuming there are N magnetic ions a spin ice material, then we have 2^N configurations. Among these, the fraction $(6/16)^{N/2}$ are spin ice. The number 6 indicate the number of configurations with two in and two out structure in a single tetrahedron. The number 16 indicate that in each tetrahedron the ions have two choices either in or out. Therefore, the total configurations is $2^N(6/16)^{N/2}=(3/2)^{N/2}$.

Term	X_1	X_2	X_3	X_4
$\vec{J}_1 \cdot \vec{J}_2$	$-\frac{1}{3}J_{1z}J_{2z}$	$-\frac{\sqrt{2}}{3}[J_{1z}(J_{2+}+J_{2-})+(J_{1+}+J_{1-})J_{2z}]$	$\frac{1}{3}(J_{1+}J_{2+}+J_{1-}J_{2-})$	$-\frac{1}{6}(J_{1+}J_{2-}+J_{1-}J_{2+})$
$\vec{J}_3 \cdot \vec{J}_4$	$-\frac{1}{3}J_{3z}J_{4z}$	$-\frac{\sqrt{2}}{3}[J_{3z}(J_{4+}+J_{4-})+(J_{3+}+J_{3-})J_{4z}]$	$\frac{1}{3}(J_{3+}J_{4+}+J_{3-}J_{4-})$	$-\frac{1}{6}(J_{3+}J_{4-}+J_{3-}J_{4+})$
$\vec{J}_1 \cdot \vec{J}_3$	$-\frac{1}{3}J_{1z}J_{3z}$	$-\frac{\sqrt{2}}{3}[J_{1z}(\varepsilon J_{3+}+\varepsilon^2 J_{3-})+(\varepsilon J_{1+}+\varepsilon^2 J_{1-})J_{3z}]$	$\frac{1}{3}(\varepsilon^2 J_{1+}J_{3+}+\varepsilon J_{1-}J_{3-})$	$-\frac{1}{6}(J_{1+}J_{3-}+J_{1-}J_{3+})$
$\vec{J}_2 \cdot \vec{J}_4$	$-\frac{1}{3}J_{2z}J_{4z}$	$-\frac{\sqrt{2}}{3}[J_{2z}(\varepsilon J_{4+}+\varepsilon^2 J_{4-})+(\varepsilon J_{2+}+\varepsilon^2 J_{2-})J_{4z}]$	$\frac{1}{3}(\varepsilon^2 J_{2+}J_{4+}+\varepsilon J_{2-}J_{4-})$	$-\frac{1}{6}(J_{2+}J_{4-}+J_{2-}J_{4+})$
$\vec{J}_1 \cdot \vec{J}_4$	$-\frac{1}{3}J_{1z}J_{4z}$	$-\frac{\sqrt{2}}{3}[J_{1z}(\varepsilon^2 J_{4+}+\varepsilon J_{4-})+(\varepsilon^2 J_{1+}+\varepsilon J_{1-})J_{4z}]$	$\frac{1}{3}(\varepsilon J_{1+}J_{4+}+\varepsilon^2 J_{1-}J_{4-})$	$-\frac{1}{6}(J_{1+}J_{4-}+J_{1-}J_{4+})$
$\vec{J}_2 \cdot \vec{J}_3$	$-\frac{1}{3}J_{2z}J_{3z}$	$-\frac{\sqrt{2}}{3}[J_{2z}(\varepsilon^2 J_{3+}+\varepsilon J_{3-})+(\varepsilon^2 J_{2+}+\varepsilon J_{2-})J_{3z}]$	$\frac{1}{3}(\varepsilon J_{2+}J_{3+}+\varepsilon^2 J_{2-}J_{3-})$	$-\frac{1}{6}(J_{2+}J_{3-}+J_{2-}J_{3+})$

Perturbation Theory: The Hamitonian is of the spin correltion function can be write as:

$$H = H_0 + H_1$$
$$H_0 = \mathcal{J}_1 X_1$$
$$H_1 = [\mathcal{J}_2 X_2 + \mathcal{J}_3 X_3 + \mathcal{J}_4 X_4]\epsilon(t)$$

$$X_1 = -\frac{1}{3}\sum_{<ij>} J_{iz}J_{jz}$$
$$X_2 = -\frac{\sqrt{2}}{3}\sum_{<ij>}[\Lambda_{s_i s_j}(J_{iz}J_{j+}+J_{jz}J_{i+})+H.C.]$$
$$X_3 = \frac{1}{3}\sum_{<ij>}[\Lambda^*_{s_i s_j}J_{i+}J_{j+}+H.C.]$$
$$X_4 = -\frac{1}{6}\sum_{<ij>}(J_{i+}J_{j-}+H.C.)$$

With $\mathcal{J}_1 < 0$, H_0 describes a spin ice, H_1 represents quantum correlations and can be treated perturbatively. Therefore, we use the interaction representation to find time dependent operators and the time evolution operator.

$$i\hbar\frac{\partial J_{Ii+}(t)}{\partial t} = \mathcal{J}_1/3 J_{Ii+}(t)\sum_{j=n.n.} J_{jz}$$
$$J_{Ii+}(t) = J_{i+}e^{-it\mathcal{J}_1/3\sum_{j=n.n.}J_{jz}}$$
$$J_{Ii-}(t) = J_{i-}e^{it\mathcal{J}_1/3\sum_{j=n.n.}J_{jz}}$$

Hence, if we want to calculate the spin correlation function of site i and j, by using the perturbation theory, we have

$$<\vec{J_{iIn}} \cdot \vec{J_{jIn'}}> = \frac{1}{Tr[\rho_0]}[Tr[\rho_0 H_0(t'')J_{1z}J_{2z}] - iTr[\rho_0(\int_t^{-\infty} H_1(t'')dt'')J_{1I}(t)J_{2I}(t')]$$
$$- iTr[\rho_0 J_{1I}(t)(\int_{t'}^{t} H_1(t'')dt'')J_{2I}(t')] - iTr[\rho_0 J_{1I}(t)J_{2I}(t')(\int_{-\infty}^{t'} H_1(t'')dt'')]]$$

Where $Tr[\rho_0]$ is the spin ice degeneracy which can be determined by using Pauling's argument.

Conclusion: From the calculation we conclude that the perturbated term X_3 and X_4 only give the spin correlation between the nearest neighbours, however, X_2 can give spin correlation to the next neighbours.

Reference:

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