ICFP M1 - QUANTUM MATTER - TD n°7 - Solutions
Spin liquids

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1 Quantum spin ice: emergent quantum electrodynamics

The pyrochlore lattice is a lattice of corner-sharing tetrahedra (see Fig. 1B). The underlying Bravais lattice is a Face Centered Cubic (FCC) lattice (see Fig. 1A), and the lattice basis is a regular tetrahedron. The unit cell is made of two tetrahedrons.

1. How many sites per unit cell are there?

There are four since a tetrahedron has four sites. We will label them 0, 1, 2, 3.

The diamond lattice is a lattice with a two-atom basis (see Fig. 1C). The underlying Bravais lattice is an FCC lattice, and, if a diamond lattice site sits at an FCC site, the second atom (other sublattice) sits a quarter of the way along the diagonal of the FCC cubic cell.

2. What lattice do the centers of the (nearest-neighbor) *bonds* of the diamond lattice form?

A pyrochlore lattice.

3. Where do the *sites* of the diamond lattice sit with respect to the *tetrahedra* of the pyrochlore lattice?

At the centers of the tetrahedra. The diamond lattice is said to be dual to the pyrochlore lattice.

Notice that

- there are two types of tetrahedra, the "up-pointing" tetrahedra and the "down-pointing" ones. This is consistent with the diamond lattice, which has *two* sites in its basis, being the dual of the pyrochlore lattice.
- the lattice decomposes into alternating kagomé (corner-sharing triangles in 2d) and triangular planes in various directions, and most importantly that the kagomé planes contain hexagons (loops of length 6), see Fig. 2.

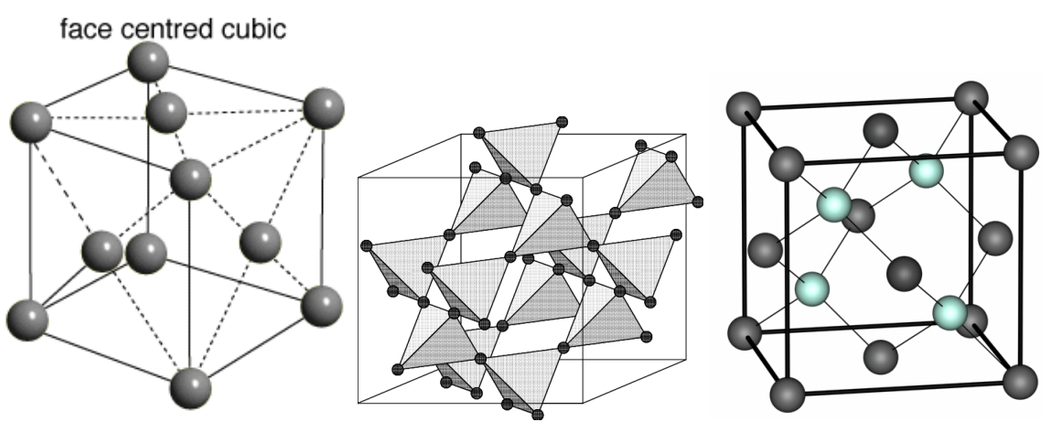

Figure 1: Some crystallographic structures. A: the face centerred cubic lattice. B: The pyrochlore lattice. C: The diamond lattice.

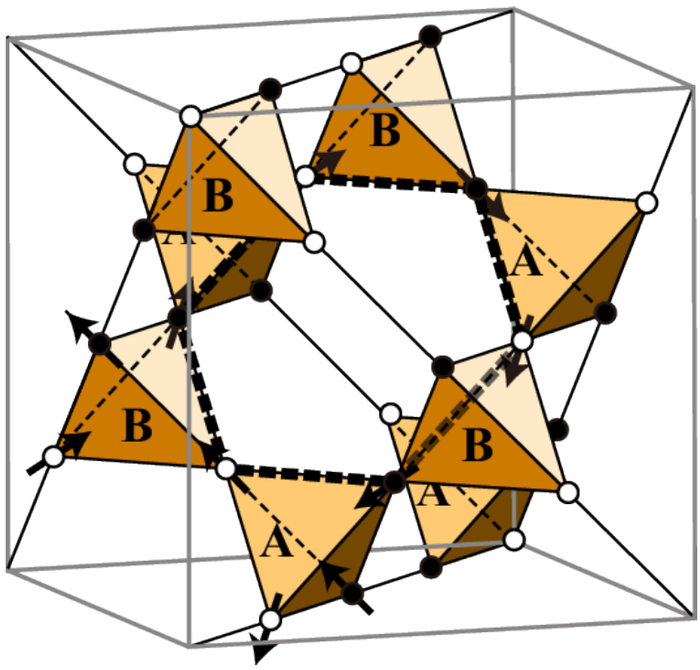

Figure 2: Hexagone loops in the pyrochlore lattice.

4. What is known as *classical* spin ice is the antiferromagnetic ($J_z > 0$) Ising model on the pyrochlore lattice. Rewrite the Ising terms on the bonds of a single tetrahedron as the square of a sum (up to a constant).

$$H = J_z \sum_{\langle ij \rangle} S_i^z S_j^z = \frac{J_z}{2} \sum_t (\sum_{i \in t} S_i^z)^2 + \text{const.} \tag{1}$$

where t is summed over the different tetrahedrons.

5. What is the condition which should be fulfilled by the ground state(s) (recall $J_z > 0$)?

We should have $\sum_{i \in t} S_i^z = 0$ for all tetrahedra, i.e.

$$S_0^z + S_1^z + S_2^z + S_3^z = 0. \tag{2}$$

6. For $S = 1/2$ find all (degenerate) ground states of a single tetrahedron.

Since $S_i^z = \pm 1/2$, this means that we want two spins up and two spins down on each tetrahedron. There are $C_4^2 = 6$ such possibilities.

7. If the tetrahedra were truly independent, what would the ground state degeneracy of a lattice of N unit cells be?

6^{2N} because there are two tetrahedra per unit cell.

We now add quantum fluctuations, *i.e.* terms in the Hamiltonian which do not commute with the Ising part. In particular, we consider "XY" or "transverse" terms:

$$H_\pm = -J_\pm \sum_{\langle ij \rangle} (S_i^+ S_j^- \pm S_i^- S_j^+). \tag{3}$$

The effective Hamiltonian in perturbation theory in small $J_\pm / J_z$ actually vanishes at first and second orders. The Hamiltonian at third order takes the form

$$H_{\text{eff}} = -K \sum_{\{i,j,k,l,m,n\}=\text{hexagon}} \left(S_i^+ S_j^- S_k^+ S_l^- S_m^+ S_n^- + \text{h.c.} \right) \tag{4}$$

8. How does K scale as a function of $J_\pm$ and J_z?

$K \sim J_\pm^3/J_z^2$ since this term is obtained at third order and K has the dimensions of J. In fact, one can show that $K = 12J_\pm^3/J_z^2$.

9. Show that indeed this Hamiltonian acts purely in the ground state manifold.

Applying $H_\pm$ once, one creates two defect tetrahedra around a hexagon. By applying it three times around the loop, the defect tetrahedra eventually "annihilate".

We will now show the relation of this to a $U(1)$ lattice gauge theory. Since the effective Hamiltonian operates within the space with $\sum_{i\in t} S_i^z = 0$, it necessarily commutes with $\sum_{i\in t} S_i^z$ for every tetrahedron t separately.

10. Where does this come from within H_{eff}?

One can carry out the calculation explicitly, but we may also notice that there is always one raising and one lowering spin operator in each tetrahedron in H_{eff}.

More formally, we may define

$$Q_t = \epsilon_t \sum_{i\in t} S_i^z \underset{0}{=} 0, \tag{5}$$

where for convenience we included the factor ϵ_t which assigns a sign that discriminates two orientations of tetrahedra: $\epsilon_t = +1(-1)$ for up (down) oriented tetrahedra. The equality on the right hand side of Eq. (5) holds in the ground state sector (as indicated by the subscript 0 on the equality sign). The "charge" Q_t commutes with H_{eff}. It follows that H_{eff} is invariant under the $U(1)$ symmetry generated by the unitary operator $U = e^{i\chi Q_t}$, for any t and any χ.

Noting that the charge Q_t is defined on the sites t of a diamond lattice (the tetrahedron centers), we can recast the effective Hamiltonian entirely as a diamond lattice gauge theory. To do so, we define

$$\begin{cases} S^\pm_{t,t'} = S^{\pm\epsilon_t}_{i(t,t')} \\ S^z_{t,t'} = S^z_{i(t,t')} \end{cases}, \tag{6}$$

where $i(t,t')$ is the pyrochlore site shared by neighboring tetrahedra t and t'. This definition gives a "vectorial" sense to the operators on the diamond lattice. Then the gauge charge becomes

$$Q_t = \epsilon_t \sum_{t'\in\partial t} S^z_{t,t'} \equiv \epsilon_t (\text{div}[S^z])_t \underset{0}{=} 0, \tag{7}$$

where the sum indicates nearest neighbor sites of t, and the result is the lattice divergence at t of the vector field $S^z_{t,t'}$. We recognize therefore $S^z_{t,t'}$ as the lattice analog of the "electric field" in Gauss' law. Let us make things even more explicit by writing things as:

$$S^z_{t,t'} \to E_{t,t'}, \qquad S^\pm_{t,t'} \to e^{\pm iA_{t,t'}}, \tag{8}$$

where $E_{t,t'}$ is a half-integral valued angular momentum, and $A_{t,t'} = -A_{t',t}$ is a 2π-periodic angular variable. If we impose the canonical commutation relations $[E_{t,t'}, A_{t,t'}] = i$ (think of $[L^z, \varphi] = i$), then $S^\pm_{t,t'}$ acts as the desired spin raising/lowering operator, except that it can raise/lower "outside" the physical space with $E_{t,t'} = \pm 1/2$.

11. Rewrite H_{eff} using Eq. (8). Defining the lattice curl as

$$(\text{curl}[A])_{\text{hexagon}} = \sum_{(t\in\text{hex})=1}^{6} A_{t,t+1} \tag{9}$$

which defines a "magnetic flux" B through a plaquette, show that H_{eff} takes the form of

$$H_{\text{eff}} = -2K \sum_{\text{hexagon}} \cos(\text{curl}[A]). \tag{10}$$

$$\begin{aligned} H_{\text{eff}} &= -K \sum_{\text{hexagon}} (e^{i(A_{1,2}-(-A_{2,3})+A_{3,4}-(-A_{4,5})+A_{5,6}-(-A_{6,1}))} + \text{h.c.}) && (11)\\ &= -2K \sum_{\text{hexagon}} \cos(A_{1,2}+A_{2,3}+A_{3,4}+A_{4,5}+A_{5,6}+A_{6,1}) && (12)\\ &= -2K \sum_{\text{hexagon}} \cos(\text{curl}[A]) && (13) \end{aligned}$$

12. Show that this Hamiltonian has a manifest gauge invariance under local phase rotations by an angle χ_t on each diamond site, for which

$$S^{\pm}_{t,t'} \to e^{\pm i(\chi_{t'}-\chi_t)} S^{\pm}_{t,t'}. \tag{14}$$

It is clear from the previous question: such a transform preserves the curl.

13. Now imposing the spin-1/2 constraint y adding a term $U(E^2 - 1/4)$ (notice that $U \to +\infty$ will project out the unphysical states), and assuming small $B = \text{curl}[A]$, show that the Hamiltonian is that of quantum electrodynamics without matter fields $H \sim E^2 + B^2$.

$$H = \frac{\tilde{U}}{2} \sum_{\langle t,t' \rangle} E^2_{t,t'} + \frac{\tilde{K}}{2} \sum_{\text{hex}} B^2, \tag{15}$$

where $\tilde{U} = 2U$, $\tilde{K} = 2 \times (-2K(-1/2)) = 2K$, since we assumed we could take $\cos(\text{curl}A) \approx 1 - (\text{curl}A)^2/2$. This is the Hamiltonian for quantum electrodynamics. It is a $U(1)$ gauge theory whose solutions we know. At low energies, there is a photon mode. Here the photon mode corresponds to fluctuations of S^z, and can indeed be seen in neutron scattering experiments through the $\langle S^z S^z \rangle$ correlations.

Remark: This describes the low energy theory, without matter fields (without "electrons" and "positrons"). To go further and include those, one instead writes $S^+_{r,r'} = \Phi^\dagger_t e^{iA_{t,t'}} \Phi_{t'}$ and S^z is unchanged, one obtains spinons (Φ) hopping in the background of fluctuating gauge fields, and the gauge transformation must include also $\Phi_t \to \Phi_t e^{-i\chi_t}$.