

ICFP M1 - QUANTUM MATTER - TD n°5 - Exercises

Spin liquids & Chern numbers

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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?

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

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).
5. What is the condition which should be fulfilled by the ground state(s) (recall $J_z > 0$)?
6. For $S = 1/2$ find all (degenerate) ground states of a single tetrahedron.
7. If the tetrahedra were truly independent, what would the ground state degeneracy of a lattice of N unit cells be?

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:

$$H_{\pm} = -J_{\pm} \sum_{\langle ij \rangle} (S_i^+ S_j^- \pm S_i^- S_j^+). \quad (1)$$

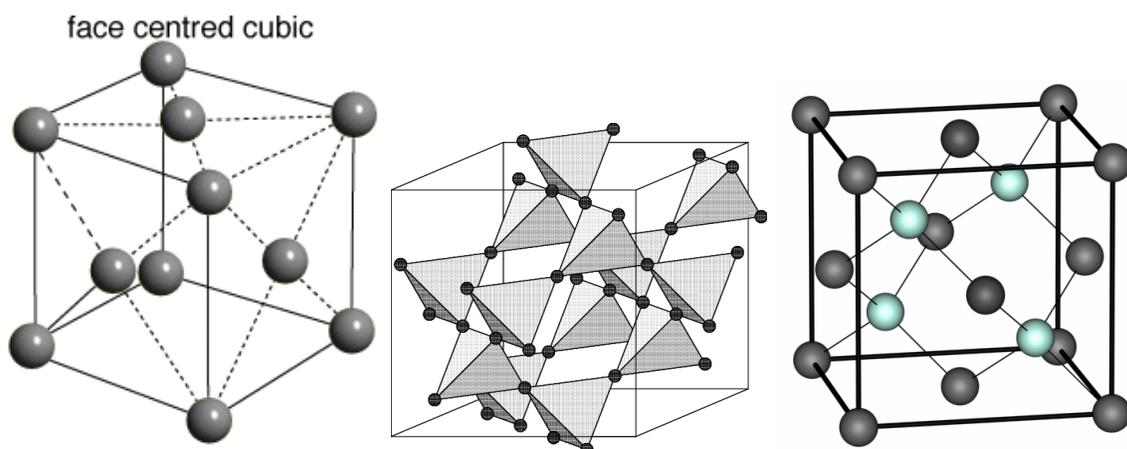


Figure 1: Some crystallographic structures. A: the face centered cubic lattice. B: The pyrochlore lattice. C: The diamond lattice.

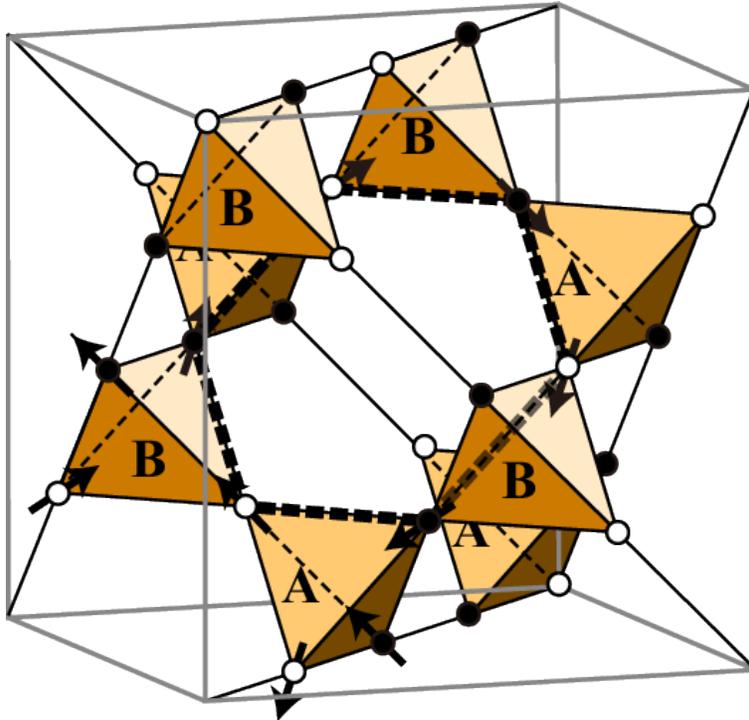


Figure 2: Hexagone loops in the pyrochlore lattice.

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

$$H_{\text{eff}} = -K \sum_{\{i,j,k,l,m,n\}=\text{hexagon}} \left(S_i^+ S_j^- S_k^+ S_l^- S_m^+ S_n^- + \text{h.c.} \right) \quad (2)$$

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

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

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} ?

More formally, we may define

$$Q_t = \epsilon_t \sum_{i \in t} S_i^z \stackrel{0}{=} 0, \quad (3)$$

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. (3) 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

$$\begin{cases} S_{t,t'}^{\pm} = S_{i(t,t')}^{\pm \epsilon_t} \\ S_{t,t'}^z = S_{i(t,t')}^z \end{cases}, \quad (4)$$

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

$$Q_t = \epsilon_t \sum_{t' \in \partial t} S_{t,t'}^z \equiv \epsilon_t (\text{div}[S^z])_t \stackrel{0}{=} 0, \quad (5)$$

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

$$S_{t,t'}^z \rightarrow E_{t,t'}, \quad S_{t,t'}^{\pm} \rightarrow e^{\pm i A_{t,t'}}, \quad (6)$$

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 $S_{t,t'}^{\pm}$ 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. (6). Defining the lattice curl as

$$(\text{curl}[A])_{\text{hexagon}} = \sum_{(t \in \text{hex})=1}^6 A_{t,t+1} \quad (7)$$

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

$$H_{\text{eff}} = -2K \sum_{\text{hexagon}} \cos(\text{curl}[A]). \quad (8)$$

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

$$S_{t,t'}^{\pm} \rightarrow e^{\pm i(\chi_{t'} - \chi_t)} S_{t,t'}^{\pm}. \quad (9)$$

13. Now imposing the spin-1/2 constraint by adding a term $U(E^2 - 1/4)$ (notice that $U \rightarrow +\infty$ 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 $H \sim E^2 + B^2$.

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

2 Berry curvature and Hall conductivity of Haldane’s honeycomb model

In class, you introduced the low-energy Hamiltonian version of the Haldane model, namely

$$H = v (\mu^z \tau^x k_x + \tau^y k_y) + m_1 \tau^z + m_2 \mu^z \tau^z, \quad (10)$$

where the Pauli matrices mean the following:

- $\tau^z = \pm 1$: sublattices A/B,
- $\mu^z = \pm 1$: valley K/K',
- $\sigma^z = \pm 1$: spin $\pm 1/2$ (H in Eq. (10) is diagonal in spin, i.e. one should think about it as being multiplied by $\sigma^0 = \text{Id}_2^{(\sigma)}$).

Using the fact that μ^z commutes with all terms in H , you found that the energy dispersions for fixed $\mu^z = \pm 1$ were

$$\epsilon_{\pm}(m_1, m_2) = \pm \sqrt{v^2 k^2 + (m_1 + \mu^z m_2)^2}. \quad (11)$$

1. Derive this and find expressions for the corresponding eigenstates.
2. Show that the gap vanishes (i.e. there exists at least one \mathbf{k}_0 such that $\epsilon_{-}(\mathbf{k}_0) = \epsilon_{+}(\mathbf{k}_0)$) if $|m_1| = |m_2|$ and in the case $\mu^z = -\text{sign}(m_1/m_2)$.

Assume that the system is “half-filled,” i.e. that the ϵ_{-} band(s) are filled, and the ϵ_{+} one(s) are empty. Recall the expression of the Berry phase of the lower band (ϵ_{-} band, also called valence band):

$$\Omega_{-}(\mathbf{k}) = \partial_x \mathcal{A}_{-}^y - \partial_y \mathcal{A}_{-}^x, \quad \text{with} \quad \mathcal{A}_{-}^{\mu}(\mathbf{k}) = i \langle u_{-\mathbf{k}} | \partial_{\mu} | u_{-\mathbf{k}} \rangle, \quad (12)$$

where $\partial_{\mu} \equiv \frac{\partial}{\partial k^{\mu}}$. We will derive an expression of the Berry curvature (which applies beyond the Haldane model) which will be easier to use than the definition Eq. (12).

3. Show that, for $n = \pm$,

$$\Omega_n(\mathbf{k}) = -2 \text{Im}[\langle \partial_x u_{n\mathbf{k}} | \partial_y u_{n\mathbf{k}} \rangle]. \quad (13)$$

4. Using $\langle u_{n\mathbf{k}} | u_{n\mathbf{k}} \rangle = 1$ and $\langle u_{n\mathbf{k}} | u_{m\mathbf{k}} \rangle = 0$ for $m \neq n$ and differentiating, show that

$$\Omega_n(\mathbf{k}) = -i \sum_{m \neq n} (\langle u_{n\mathbf{k}} | \partial_x u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | \partial_y u_{n\mathbf{k}} \rangle - \langle u_{n\mathbf{k}} | \partial_y u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | \partial_x u_{n\mathbf{k}} \rangle) \quad (14)$$

5. Show that

$$\Omega_n(\mathbf{k}) = i \sum_{m \neq n} \left(\frac{\langle u_{n\mathbf{k}} | \partial_x H | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | \partial_y H | u_{n\mathbf{k}} \rangle - \langle u_{n\mathbf{k}} | \partial_y H | u_{m\mathbf{k}} \rangle \langle u_{m\mathbf{k}} | \partial_x H | u_{n\mathbf{k}} \rangle}{(E_n(\mathbf{k}) - E_m(\mathbf{k}))^2} \right). \quad (15)$$

To do so, write Schrödinger’s equation for a band n

$$H | u_{n\mathbf{k}} \rangle = E_n(\mathbf{k}) | u_{n\mathbf{k}} \rangle, \quad (16)$$

contract it on the left with the eigenstate for a band m

$$\langle u_{m\mathbf{k}} | H | u_{n\mathbf{k}} \rangle = E_n(\mathbf{k}) \langle u_{m\mathbf{k}} | u_{n\mathbf{k}} \rangle, \quad (17)$$

and differentiate with respect to k_{μ} .

6. Let us now go back to the specific case of the Haldane model. Writing $H = v\mu^z\tau^x k_x + v\tau^y k_y + m\tau^z$ (think $m = m_1 + \mu^z m_2$) and noticing that

$$|u_{\pm\mathbf{k}}\rangle\langle u_{\pm\mathbf{k}}| = \frac{1}{2} \left(\tau^0 \pm \frac{H}{\epsilon_{+\mathbf{k}}} \right), \quad (18)$$

recover the result for the Berry phase of the lower band of the Haldane model given in class, i.e.

$$\Omega_-(\mathbf{k}) = \mu^z \frac{mv^2}{2(v^2k^2 + m^2)^{3/2}}. \quad (19)$$

7. What is the sign of $\Omega_+(\mathbf{k})$ compared to that of $\Omega_-(\mathbf{k})$?

8. Check that

$$\int d^2k \Omega_-(\mathbf{k}) = \pi\mu^z \text{sign}(m). \quad (20)$$

To do so, extend the integral over the BZ to infinity and recall $\int_0^\infty dx x/(x^2 + b^2)^{3/2} = 1/\sqrt{b^2}$.

9. Note the appearance of μ^z . This appears because the valley determines the sense of winding of the Dirac point, or chirality. For a given sign of mass, opposite chirality gives opposite Berry curvature. The integrand is strongly peaked in a region of width m/v in momentum space around the Dirac point. So when the Fermi level lies in the gap formed by the mass, we can say, using the general formula $C_n = \frac{1}{2\pi} \int_{\text{BZ}} d^2k \Omega_n(\mathbf{k})$, that each Dirac point contributes plus or minus half an integer to the Chern number. This must be added for every distinct Dirac point, i.e. for each spin and valley. Therefore there is a general formula for the Chern number for a set of massive Dirac points with the Fermi level in the gap:

$$C = \sum_i \frac{1}{2} \text{sign}(m_i \mu_i^z) \quad (21)$$

Here the sum is over all Dirac points, i.e. for our model of graphene it includes four such points, for spin and valley. One might be worried about Eq. (21), because it looks like it can give a half-integer quantum Hall effect. However, for any physical two dimensional system, there is a famous theorem (Nielsen-Ninomiya) that there must always be an even number of Dirac points. This guarantees an integer result for an insulator.

10. Let's apply the formula Eq. (21) to two limit cases.

- (a) Apply Eq. (21) in the limit $m_2 = 0$.
 (b) Now consider the limit $m_1 = 0$.

Remark: Can these insulators be distinguished experimentally? Yes! The nontrivial ($C \neq 0$ in this case) insulators have edge states and a nonzero (and quantized) Hall conductivity, which the "trivial" ($C = 0$ here) insulators do not have. In fact, one can show that

$$C = N_R - N_L, \quad (22)$$

where N_R and N_L are the number of "right" and "left" movers respectively at a boundary. This is an instance of the "bulk-boundary correspondence";

$$\sigma_H = \frac{\sigma_{yx} - \sigma_{xy}}{2} = e^2 \sum_{n \text{ occupied}} \int \frac{d^2k}{(2\pi)^2} \Omega_n(\mathbf{k}) = \frac{e^2}{2\pi} \sum_{n \text{ occupied}} C_n = \frac{e^2}{h} C, \quad (23)$$

where we restored the factor \hbar to get physical units. This is the TKNN formula. (One can also understand it from the bulk-boundary correspondence.) We have therefore shown that one can have a nonzero Hall conductivity in the absence of a magnetic field.