Lecture 12: Expanding the Berry phase term

In this lecture, we will pick up the threads from where we left off last time, and use the decomposition of $\vec{N}$ into an alternating Neel part $\hat{n}$ and a uniform part $\vec{L}$ to rewrite the Berry phase term in a more useful and transparent way.

In principle, we have to simply take

$$S_B \;\; = \;\; \int_0^\beta d\tau \sum_i iS \int_0^1 du\, \vec{N}(\vec{r}_i, u, \tau) \cdot \left(\frac{\partial \vec{N}(\vec{r}_i, u, \tau)}{\partial u} \times \frac{\partial \vec{N}(\vec{r}_i, u, \tau)}{\partial \tau}\right),$$

$$(1)$$

insert the decomposition

$$\vec{N}(\vec{r}_j, \tau) \;\; = \;\; \eta(\vec{r}_j)\hat{n}(\vec{r}_j, \tau)\sqrt{1 - (a^d/S)^2 \vec{L}^2} + \frac{a^d}{S}\vec{L}(\vec{r}_j, \tau), \qquad (2)$$

and expand out the answer using the slowly varying nature of $\hat{n}$ and the smallness of $\vec{L}$

However, at a formal level, we need to first understand how to "extend" the $\hat{n}$ and $\vec{L}$ defined at $u = 1$ (*i.e.* for the physical configurations) to the entire interval $0 \leq u \leq 1$. To understand this, we first note that $\vec{N}(u, \tau)$ is defined as the vector obtained by rotating $\hat{z}$ by $u\theta(\vec{N}(\tau))$ instead of the "physical" angle $\theta(\vec{N}(\tau))$, but about the *same axis* $\vec{M}(\vec{N}(\tau))$ (we have dropped the $\vec{r}_i$ dependence for ease of notation). With this in mind, we can decompose $\vec{N}(\vec{r}_i, u, \tau)$ using the same prescription we used earlier for $\vec{N}(\vec{r}_i, \tau)$, *i.e.* by coarse-graining a configuration of $\vec{N}(\vec{r}_i, u, \tau)$ over a length scale l of order a few lattice spacings a to define a local direction $\hat{n}(\vec{r}, u, \tau)$ and taking components of $\vec{N}(\vec{r}_i, u, \tau)$ along and perpendicular to $\hat{n}(\vec{r}, u, \tau)$. In other words, we have the decomposition

$$\vec{N}(\vec{r}_j, u, \tau) \;\; = \;\; \eta(\vec{r}_j)\hat{n}(\vec{r}_j, u, \tau)\sqrt{1 - (a^d/S)^2 \vec{L}^2} + \frac{a^d}{S}\vec{L}(\vec{r}_j, u, \tau)$$
$$\text{with } \;\; \hat{n}(\vec{r}_j, u, \tau) \cdot \vec{L}(\vec{r}_j, u, \tau) \;\; = \;\; 0$$

$$(3)$$

With this in mind, we can go ahead with the expansion of S_B. This expansion will result in four kinds of terms, classified by the number of places in which $\vec{N}$ is replaced by the alternating part (in the rest, it is replaced by

the uniform part). Of these, the term with all $\vec{N}$ replaced by the uniform part is clearly a higher order effect, given that it involves three powers of $\vec{L}$. The term with two $\vec{N}$ replaced by their uniform parts and one by its alternating part has an overall factor of $\eta(\vec{r}_i)$ in front, and the oscillatory nature of this factor implies again that this term is a small higher order effect which can be neglected.

We are thus left with two kinds of terms. One is obtained by replacing all three $\vec{N}$ by their alternating parts. To leading order, one can set the *magnitude* of the alternating part to one, *i.e.* use the zeroth order term in the expansion of the square-root in powers of $\vec{L}$, to obtain

$$ S'_B \;\; = \;\; iS \sum_j \eta(\vec{r}_j) \mathcal{A}_z(\hat{n}(\vec{r}_j, \tau)) \; , $$

(4)

i.e. the alternating sum of the signed areas $\mathcal{A}_z$ subtended on the unit sphere by $\hat{n}(\vec{r}_j, \tau)$ as τ is varied from 0 to β. This is a tricky term to handle due to its oscillatory nature, and we will come back to it later.

The second set of terms that survive all have one field replaced by its uniform part and two replaced by their alternating parts. No oscillatory factors $\eta(\vec{r}_j)$ appear due to the even number of alternating parts. Apart from a boundary contribution (see below) whose correct magnitude requires us to keep track of the *magnitude* of the alternating part, we can again set each square root to one, and write these terms as:

$$ \frac{a^d}{S} iS \sum_j \int_0^\beta d\tau \int_0^1 du \left[\hat{n} \cdot \left(\frac{\partial \vec{L}}{\partial u} \times \frac{\partial \hat{n}}{\partial \tau} \right) + \vec{L} \cdot \left(\frac{\partial \hat{n}}{\partial u} \times \frac{\partial \hat{n}}{\partial \tau} \right) + \hat{n} \cdot \left(\frac{\partial \hat{n}}{\partial u} \times \frac{\partial \vec{L}}{\partial \tau} \right) \right] $$

(5)

The second term in the square bracket above is zero because the cross product

$$ \frac{\partial \hat{n}}{\partial u} \times \frac{\partial \hat{n}}{\partial \tau} $$

is a cross product of two vectors both of which are perpendicular to $\hat{n}(\vec{r}_j, u, \tau)$, and therefore must lie *along* $\hat{n}(\vec{r}_j, u, \tau)$, *i.e.* perpendicular to $\vec{L}(\vec{r}_j, u, \tau)$.

The other two terms that survive can be rewritten as

$$ \frac{a^d}{S} iS \sum_j \int_0^\beta d\tau \int_0^1 du \left(\frac{\partial}{\partial \tau} \left[\hat{n} \cdot \frac{\partial \hat{n}}{\partial u} \times \vec{L} \right] + \frac{\partial}{\partial u} \left[\hat{n} \cdot \vec{L} \times \frac{\partial \hat{n}}{\partial \tau} \right] \right) $$

(6)

2

Written in this form, it is clear that the first term, being a total derivative with respect to τ, is zero due to the periodic boundary conditions in the τ direction. The second term, being a total derivative with respect to u, can be written in terms of the boundary contributions at $u = 1$ and $u = 0$:

$$iS \sum_j \int_0^\beta d\tau \left(\hat{n} \cdot \vec{L} \times \frac{\partial \hat{n}}{\partial \tau} \right) \Big|_{u=0}^{u=1} \tag{7}$$

Now, we note that the contribution from $u = 0$ vanishes to this order. The argument is as follows: We observe that

$$\vec{N}(\vec{r}_j, u = 0, \tau) = \hat{z} \tag{8}$$

since the rotation angle is zero. As a result, *the magnitude of the alternating part goes to zero as $u \to 0$*. Therefore, we need to remember that our analysis of this set of terms was performed under the assumption that

$$\sqrt{1 - (a^{2d}/S^2)\vec{L}^2} \tag{9}$$

remained close to 1, and go back and keep track of this factor more carefully, especially in the step in which we rewrite the term as an integral of total derivatives. This is a straightforward but notationally cumbersome exercise, which tells us that the boundary contribution from $u = 0$ vanishes to this order (you should check this!) since there is no alternating part at all at $u = 0$.

Therefore, we are left with (in continuum notation)

$$-i \int_\Lambda d^d x \int_0^\beta d\tau \vec{L} \cdot \left(\hat{n} \times \frac{\partial \hat{n}}{\partial \tau} \right) \tag{10}$$

Thus, we have shown that the Berry phase term S_B can be rewritten to leading order as a sum of two contributions:

$$
\begin{aligned}
S_B &= S_B' - i \int_\Lambda d^d x \int_0^\beta d\tau \vec{L} \cdot \left(\hat{n} \times \frac{\partial \hat{n}}{\partial \tau} \right) , \\
S_B' &= iS \sum_j \eta(\vec{r}_j) \mathcal{A}_z(\hat{n}(\vec{r}_j, \tau)) .
\end{aligned}
\tag{11}
$$

Here, we have written the second term in continuum notation to emphasize that lattice level details do not enter into its formulation, while the first term,

3

which depends exclusively on $\hat{n}$, is of course an alternating lattice sum that cannot be coarse-grained without losing information.

Our partition function can now be written as a functional integral over configurations of $\vec{L}$ and $\hat{n}$, instead of over configurations of the original $\vec{N}$. In other words, we have

$$
Z \;=\; \int_{\hat{n}^2=1} \mathcal{D}\hat{n}\mathcal{D}\vec{L}\,\delta(\vec{L}\cdot\hat{n})\exp\left(S_B'(\hat{n}) - \int_0^\beta d\tau \int_\Lambda d^d x \right.
$$
$$
\left. \left[\frac{\rho_s}{2}(\nabla n)^2 + \frac{\vec{L}^2}{2\chi_\perp} + i\vec{L}\cdot\left(\hat{n}\times\frac{\partial\hat{n}}{\partial\tau} \right) \right] \right)
$$
$$(12)$$

At this point, let us temporarily ignore the presence of $S_B'(\hat{n})$ and develop some feeling for the rest of this functional integral expression, *i.e.* ask: What system's partition function is described by this formula in the absence of $S_B'(\hat{n})$? To answer this, consider a spatial lattice with lattice spacing $\Lambda^{-1} \sim l$, the coarse-graining scale. At each point of this lattice, there is a unit vector $\hat{n}$. There is an energetic cost to neighbouring unit vectors being out of alignment—this is captured by the stiffness ρ_s. This energy functional is simply that of a classical ferromagnetic $O(3)$ model, in which nearest neighbour "spins" (unit 3-vectors) like to be aligned. Quantum mechanics enters through the kinetic energy for these unit vectors. Thinking of each unit vector as the position of a fictitious particle of mass $\chi_\perp$ on the corresponding unit sphere (in spin space), it is clear that the kinetic energy must be the square of the corresponding angular momentum vector divided by two times the mass of the partice. Since the Newtonian mechanics expression for $\vec{L}$ is

$$
\vec{L} \;=\; \chi_\perp\left(\hat{n}\times\frac{\partial\hat{n}}{\partial\tau} \right)
$$
$$(13)$$

and the kinetic energy is

$$
\frac{1}{2\chi_\perp}\vec{L}^2
$$
$$(14)$$

it is clear that $\vec{L}$ must be perpendicular to $\hat{n}$, and that the *phase space path integral* for the partition function of such a system would take on exactly the same form as our path integral expression for Z if we ignore the S_B' term.

Thus, without the S'_B term, our expression describes the partition function of $O(3)$ *quantum rotors* with moment of inertia $\chi_\perp$ and aligning interactions controlled by ρ_s.

In other words, the *Hamiltonian* formulation of this system of quantum rotors (ignoring $S'_B(\hat{n})$) is

$$
\begin{aligned}
H_{\text{rotor}} &= \int d^d x \left(\frac{\vec{L}^2}{2\chi_\perp} + \frac{\rho_s}{2} (\nabla \hat{n})^2 \right) \\
[n_\alpha(\vec{r}), L_\beta(\vec{r}')] &= i\delta^d(\vec{r} - \vec{r}')\epsilon^{\alpha\beta\gamma} n_\gamma(\vec{r}) \\
[L_\alpha(\vec{r}), L_\beta(\vec{r}')] &= i\delta^d(\vec{r} - \vec{r}')\epsilon^{\alpha\beta\gamma} L_\gamma(\vec{r})
\end{aligned}
\tag{15}
$$

where the commutators listed above tell us that the $\vec{L}$ are now the angular momentum operators that are canonically conjugate to the positions $\hat{n}$.

With that in mind, we can write down the coordinate-space path integral for this quantum rotor model by integrating over the $\vec{L}$ in the earlier phase-space path integral representation. This is straightforward to do by introducing a Lagrange multiplier field λ to take care of the orthogonality constraint:

$$
\prod_{\vec{r},\tau} \delta(\vec{L} \cdot \hat{n}) = \int \mathcal{D}\lambda e^{-i \int d^d x \int_0^\beta d\tau \lambda (\vec{L} \cdot \hat{n})}
\tag{16}
$$

The $\vec{L}$ functional integral is now a simple Gaussian integral and can be performed by completing the square in the exponential, after which the λ functional integral can be done to enforce the orthogonality constraint:

$$
\begin{aligned}
&\int \mathcal{D}\lambda \int \mathcal{D}\vec{L} \exp\left(-\int d^d x \int_0^\beta d\tau [\frac{\vec{L}^2}{2\chi_\perp} + i\vec{L} \cdot (\hat{n} \times \frac{\partial \hat{n}}{\partial \tau} + \lambda \hat{n})] \right) \\
&= \text{const.} \int \mathcal{D}\lambda \exp\left(-\frac{\chi_\perp}{2} \int d^d x \int_0^\beta d\tau (\hat{n} \times \frac{\partial \hat{n}}{\partial \tau} + \lambda \hat{n})^2 \right) \\
&= \text{const.} \exp\left(-\frac{\chi_\perp}{2} \int d^d x \int_0^\beta d\tau \, (\frac{\partial \hat{n}}{\partial \tau})^2 \right) \int \mathcal{D}\lambda \exp\left(-\frac{\chi_\perp}{2} \int d^d x \int_0^\beta d\tau \, \lambda^2 \right) \\
&= \text{const}' \exp\left(-\frac{\chi_\perp}{2} \int d^d x \int_0^\beta d\tau \, (\frac{\partial \hat{n}}{\partial \tau})^2 \right)
\end{aligned}
\tag{17}
$$

In other words, we have demonstrated that the low-energy effective theory for a system with short range antiferromagnetic order can be written as:

$$Z \quad \propto \quad \int_{\hat{n}^2=1} \mathcal{D}\hat{n} \exp\left(S'_B(\hat{n}) - \frac{\rho_s}{2} \int_0^\beta d\tau \int d^d x ((\nabla\hat{n})^2 + \frac{1}{c^2}(\frac{\partial\hat{n}}{\partial\tau})^2) \right)$$

$$(18)$$

where we have introduced the *velocity c*

$$c \quad \equiv \quad \sqrt{\frac{\rho_s}{\chi_\perp}}$$
$$\sim \quad JSa \qquad (19)$$

which converts between space and imaginary time dimensions.

Rescaling $\tau \to c\tau$ and $\beta \to c\beta$, we can rewrite the action as

$$S \quad = \quad S'_B + \frac{1}{2g} \int_0^{\beta c} d\tau \int d^d x ((\nabla\hat{n})^2 + (\frac{\partial\hat{n}}{\partial\tau})^2)$$
$$\text{where} \quad g \quad = \quad \sqrt{\frac{1}{\chi_\perp \rho_s}} \quad \sim \quad \frac{a^{d-1}}{S} \qquad (20)$$

As we will see later, although we do not know its value precisely, c is really a velocity, in the sense that it controls the velocity of certain wavelike excitations in the antiferromagnetic phase. Nor do we know the values of g or Λ precisely, and of course they are not measurable quantities since both depend on our choice of coarse-graining procedure.

How then are we to use such an effective theory? For concreteness, consider the case in which the theory describes a gapped phase, with energy gap Δ separating the ground state from excited states—note that Δ can be measured via its effect on the specific heat, for instance. Now, the way one can use the effective theory is to compute Δ as a function of Λ, c and g. As we shall see later, one can then calculate any other physical property and remove all explicit mention of g and Λ in the final answer by re-expressing the answer as a function of Δ, c, and T. In this way, we can use this effective theory to get results for other observables in terms of the measured gap in the spectrum—these are *testable predictions*.

To do any of these calculations, we need to know what quantity in the effective theory plays the role of a particular microscopic observable.

6

The answer is already clear from our derivation of this effective theory: Namely, Fourier components $\vec{S}(\vec{k})$ of the spin density operator at $\vec{k} = \mathbf{Q} + \vec{q}$ and q small are represented by S times the corresponding Fourier components $\hat{n}(\vec{q})$ of the $\hat{n}$ field, while the Fourier components $\vec{S}(\vec{q})$ of the spin density operator at small q near zero wavevector are represented by the corresponding Fourier components $\vec{L}(\vec{q})$ of the $\vec{L}$ field:

$$
\begin{aligned}
\vec{S}[\mathbf{Q} + \vec{q}] &\sim S\hat{n}(\vec{q}) \, , \quad q \text{ small} \\
\vec{S}[\vec{q}] &= \vec{L}(\vec{q}) \, , \quad q \text{ small} \, .
\end{aligned}
$$
(21)

Here, $\mathbf{Q}$ is the antiferromagnetic ordering wavevector at which the Fourier transform of $\eta(\vec{r})$ is concentrated, In the next class, we will quickly summarize the effects of S'_B and then discuss experimental probes of antiferromagnets, so that we have an idea of the types of quantities one would be interested in calculating with such an effective theory.