Lecture 13: Berry phase effects in $d = 1$ and $d = 2$ antiferromagnets

Before we discuss the physics of standard experimental probes of quantum antiferromagnetism, we have some unfinished business from the last lecture, namely, the term S'_B in the effective theory for quantum antiferromagnets, and the role it plays in determining the low energy physics. Let us first focus on $d = 1$, *i.e.* the case of an *antiferromagnetic spin chain* with spin S moments arranged along a one dimensional lattice and interacting with nearest neighbours via an antiferromagnetic exchange interaction J. Such a model Hamiltonian, for $S = 1/2$, describes "cousins" of La_2CuO_4, in which the Copper and Oxygen atoms are arranged in such a way that the Copper moments form one dimensional chains, instead of two-dimensional square-lattices like in the case of La_2CuO_4. Other examples include certain Nickel, Vanadium and Chromium oxides, in which these ions form chains of $S = 1$ or $S = 3/2$ moments that are coupled antiferromagnetically. As in the case of La_2CuO_4, this exchange coupling between nearest neighbours is far bigger in magnitude than the usual dipolar interaction between two magnetic dipoles, and therefore, we ignore this dipolar interaction in all our analysis.

With all of this in mind, we consider such a chain of L sites with periodic boundary conditions and L even, and note that we can rewrite S'_B in $d = 1$ in the following suggestive way, which has an immediate geometric interpretation:

$$S'_B = iS \sum_{j=1}^{L/2} (\mathcal{A}_z(\hat{n}(\vec{r}_{2j}, \tau)) - \mathcal{A}_z(\hat{n}(\vec{r}_{2j-1}, \tau)) \; , \tag{1}$$

with understanding that $\hat{n}(\vec{r}_L, \tau) \equiv \hat{n}(\vec{r}_0, \tau)$. The geometric interpretation alluded to above is easy to understand (see Fig 1). Each term represents the(signed) area of the strip *between* the trajectories inscribed by $\hat{n}(\vec{r}_{2j}, \tau)$ and $\hat{n}(\vec{r}_{2j-1}, \tau)$ as τ is varied from 0 to β. When we add up all these little strips of area, what do we get? To answer this, we use this geometric interpretation to remove all reference to the internal coordinate u that we needed to use to represent each $\mathcal{A}$ explicitly, and write this term more transparently as

$$iS \sum_{j=1}^{L/2} (\mathcal{A}_z(\hat{n}(\vec{r}_{2j}, \tau)) - \mathcal{A}_z(\hat{n}(\vec{r}_{2j-1}, \tau)) \quad =$$

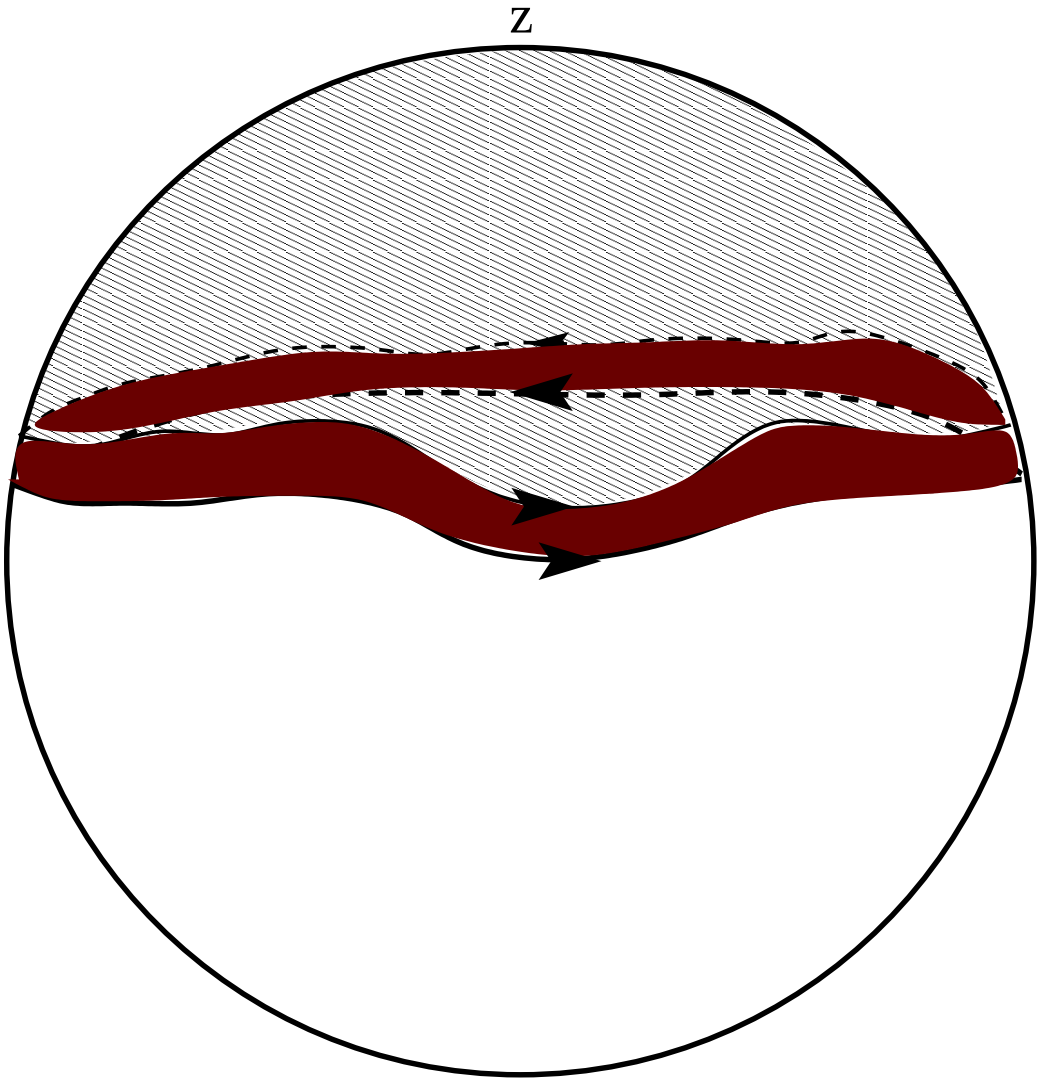

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Figure 1: The brown strip represents the *difference* between the signed areas swept by successive $\hat{n}$ along the chain. One can write down a formula for its area without the need to invoke the *internal coordinate* u like we needed to do earlier for the area of the spherical cap swept by any one $\hat{n}$.

$$\frac{iS}{2}(2a)\sum_{j=1}^{L/2}\int_0^\beta d\tau\hat{n}\cdot\left(\frac{\Delta\hat{n}(\vec{r}_{2j},\tau)}{a}\times\frac{\partial\hat{n}}{\partial\tau}(\vec{r}_{2j},\tau)\right) \tag{2}$$

where

$$\Delta\hat{n}(\vec{r}_{2j},\tau) \;=\; \hat{n}(\vec{r}_{2j},\tau)-\hat{n}(\vec{r}_{2j-1},\tau) \tag{3}$$

and we have multiplied and divided by a factor of 2 as well as by a factor of a to emphasize that this can be viewed as the discrete approximation to the following continuum formula, valid if the variation of $\hat{n}$ is slow:

$$+\frac{iS}{2}\int_0^L dx\int_0^\beta d\tau\hat{n}\cdot\left(\frac{\partial\hat{n}}{\partial x}\times\frac{\partial\hat{n}}{\partial\tau}\right) \tag{4}$$

Of course there is a sign ambiguity arising from the arbitrariness in our choice of pairing, for we could equally well have written:

$$S'_B \;=\; -iS\sum_{j=0}^{L/2-1}\left(\mathcal{A}_z(\hat{n}(\vec{r}_{2j+1},\tau))-\mathcal{A}_z(\hat{n}(\vec{r}_{2j},\tau))\right), \tag{5}$$

which would have led us to the expression

$$-\frac{iS}{2}\int_0^L dx\int_0^\beta d\tau\hat{n}\cdot\left(\frac{\partial\hat{n}}{\partial x}\times\frac{\partial\hat{n}}{\partial\tau}\right) \tag{6}$$

Given this sign ambiguity, why should we trust either answer?

The answer is that the integral

$$\int_0^L dx\int_0^\beta d\tau\hat{n}\cdot\left(\frac{\partial\hat{n}}{\partial x}\times\frac{\partial\hat{n}}{\partial\tau}\right) \tag{7}$$

basically counts how many times (with signs) $\hat{n}(x,\tau)$ covers the unit sphere when x and τ range over the torus defined by the periodic boundary conditions we have imposed. Therefore, this integral must equal an *integer multiple* of 4π, say $4\pi m$.

Therefore, our result for S'_B (including the sign ambiguity) reads

$$\begin{aligned} S'_B &= \pm\frac{iS}{2}4\pi m \\ &= \pm 2\pi iSm \end{aligned} \tag{8}$$

Since S is half integer, the sign ambiguity does not affect the exponential of S'_B:

$$\exp(S'_B) \;=\; (-1)^{2mS} \; . \tag{9}$$

This suggests that our analysis, although not really rigorous, does give the right answer, and a more sophisticated treatment (outside the scope of these lectures) confirms this.

An interesting consequence of this result is that spin chains with S an integer do not feel the effects of this term since

$$\exp(S'_B) \;=\; +1 \;\; \text{for all spacetime configurations.} \tag{10}$$

Therefore, the low energy effective theory for integer spin chains is simply the quantum rotor model we wrote down in the last lecture. On the other hand, if S is equal to $1/2$ or $3/2$ or half of any odd integer, then $\exp(S'_B)$ has a dramatic effect on the path integral, since some configurations of $\hat{n}$ come with a phase factor of -1 while others do not (depending on the covering number m of that configuration):

$$\exp(S'_B) \;=\; (-1)^{m[\hat{n}]} \tag{11}$$

This distinction is at the root of the strikingly different behaviour of integer and half-integer spin chain compounds. In the integer case, as we shall see later, the system has a paramagnetic ground state in which quantum fluctuations overwhelm the classical tendency to order antiferromagnetically. Excitations above this ground state have a sizeable energy gap Δ, and it will be one of the high points of the subsequent lectures to understand how this gap is generated and how it depends on S. This gap goes under the name of the "Haldane gap" after F. D. M. Haldane who first furnished arguments connecting the behaviour of one-dimensional integer spin quantum antiferromagnets to the one dimensional quantum rotor model, and understood the resulting behaviour of the system. In contrast, half-integer spin chains are "almost" Neel ordered, in the sense that the ground state has slowly decaying power-law antiferromagnetic correlations.

Establishing this last statement is outside the scope of our lectures, since it is a subtle effect of the Berry phases which invalidate a direct connection

to the quantum rotor model—indeed, the most reliable analysis of the half-integer case proceeds quite differently, and uses the technique of "bosonization" to arrive at a low energy description which maps the system to an interacting quantum fluid of bosonic particles. We will not explicitly discuss this description in our lectures, but the analysis is actually very similar to our discussion (later in the course) of superfluidity in one dimensional quantum systems of bosons at $T = 0$ or two dimensional systems at nonzero temperature.

What about $d > 1$? Again, a detailed discussion is outside the scope of these lectures. But the basic result is that S'_B does not give rise to any non-trivial phase factors in the antiferromagnetic phase even in the half-integer case. The basic idea is that this is because the the spatial variation of $\hat{n}$ is slow: If we think of the d dimensional system as being made up of a $d-1$ dimensional array of one dimensional chains, then the fact that $\hat{n}$ is slowly varying, and the fact that the contribution of each chain is a topologically invariant integer, implies that the effects of neighbouring chains will "cancel" each other, thus ensuring that there are no non-trivial phase factors.

Of course, if we add perturbations to the Hamiltonian that drive the system away from the antiferromagnetic phase, then defects in the antiferromagnetic phase, with rapid variations of $\hat{n}$ on the scale of a lattice spacing, can certainly give rise to Berry phases. Therefore, such phase factors can be very important in the vicinity of quantum phase transitions out of the antiferromagnetic phase.

An example of this is the transition from the Neel ordered antiferromagnet on the square lattice to a so-called "valence-bond solid" (VBS) state which spontaneously breaks the lattice symmetries of the square lattice. In this VBS state, the spins are not ordered. But the "bond-energy operators" $\vec{S}_i \cdot \vec{S}_j$ on each link $\langle ij \rangle$ of the square lattice develop spatial order. In other words, their expectation value is no longer the same on all links—the system spontaneously chooses a pattern of links on which this bond energy is larger than on the rest.

It is now believed that such a transition from Neel to VBS states on the square lattice is generically driven by the proliferation of certain defect configurations that start dominating the path integral. These configurations look like "hedgehogs" centered at some space-time point—in other words $\hat{n}(\vec{r}, \tau)$ points "radially outwards" all around the center of such a hedgehog. A difficult calculation of Haldane's shows that each such hedgehog introduces a Berry phase in the path integral—this is not in violation of our argument

earlier about the absence of Berry phases, since these hedgehogs are singular objects with rapid variation of $\hat{n}$ on the lattice scale. This phase can take on one of 4 values: 1, i, -1, or $-i$ depending on the position of the core of the hedgehog. The four values correspond to the four sublattices of spatial plaquettes on top of which the core can sit, and these phases play a crucial role in the theory of this transition between Neel order and VBS order. A more detailed discussion is outside the scope of these lectures, but you can loop up the literature on "deconfined criticality" to learn more, since you are now equipped with all the prerequisites for understanding this literature.