# Lecture 9: Path integral for spin systems: Berry Phase

The path integral formulation derived in the previous lecture illustrates a point made in the last-but-one lecture—namely, there can be situations in which the weight of a path is not real and positive, due to the presence of Berry phases. The first term in the exponential in the foregoing formula, *i.e.*

$$S_B = -\int_0^\beta d\tau \sum_i \langle \vec{N}(\vec{r}_i,\tau)|\frac{d}{d\tau}\vec{N}(\vec{r}_i,\tau)\rangle \; , \tag{1}$$

is an example of such a Berry phase, since it is actually a *purely imaginary* term.

To see this, note that

$$\begin{aligned} S_B^\star &\equiv -\int_0^\beta d\tau \sum_i \left(\langle \vec{N}(\vec{r}_i,\tau)|\frac{d}{d\tau}\vec{N}(\vec{r}_i,\tau)\rangle\right)^\star \\ &= -\int_0^\beta d\tau \sum_i \langle \frac{d}{d\tau}\vec{N}(\vec{r}_i,\tau)|\vec{N}(\vec{r}_i,\tau)\rangle \\ &= +\int_0^\beta d\tau \sum_i \langle \vec{N}(\vec{r}_i,\tau)|\frac{d}{d\tau}\vec{N}(\vec{r}_i,\tau)\rangle \\ &= -S_B \end{aligned} \tag{2}$$

where we have used the fact that

$$\frac{d}{d\tau}\left(\langle \vec{N}(\tau)|\vec{N}(\tau)\rangle\right) = 0 \tag{3}$$

to obtain the penultimate equality.

In other words, $S_B$ is purely imaginary, and contributes only a phase to the weight of every path. Clearly, for this path integral formulation to be useful, it is necessary to have some understanding of just how $S_B$ attaches a phase factor to every path, *i.e.* what aspect of the path controls the corresponding phase factor.

This is what we turn to next, returning to the case of a single spin problem to illustrate the main points.

We begin by rewriting $S_B$ in a more explicit form by noting that

$$\langle \vec{N}(\tau)|\frac{d}{d\tau}\vec{N}(\tau)\rangle \;=\; \langle\psi_z|e^{+i\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}}(\frac{d}{d\tau}e^{-i\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}})|\psi_z\rangle \tag{4}$$

to obtain

$$S_B = -\int_0^\beta d\tau\langle\psi_z|e^{+i\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}}(\frac{d}{d\tau}e^{-i\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}})|\psi_z\rangle \tag{5}$$

So the main difficulty lies in computing the time derivative

$$\frac{d}{d\tau}e^{-i\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}} \tag{6}$$

when the operator in the exponential does not commute at different times. To overcome this difficulty, we need to develop a formula that generalizes the chain rule of differentiation of ordinary functions to operator-valued functions, specifically, to exponentials of operators, *i.e.* expressions of the form

$$\exp(O(\tau)) \;, \tag{7}$$

where $O(\tau)$ is an operator that depends on $\tau$ in a non-trivial way and does not commute at different times.

We do this in the following way: Consider writing

$$\exp(O(\tau)) \;=\; \underbrace{e^{\epsilon O(\tau)}\;\ldots\;e^{\epsilon O(\tau)}}_{M} \quad \text{with} \quad M\epsilon = 1 \tag{8}$$

where we have simply written the original exponential as a product of a very large number ($M$) of identical factors. Now, since each factor in this product is an exponential of an operator that is only infinitesimally different from 0 (due to the prefactor of $\epsilon$), we do not need to worry about $\epsilon O(\tau)$ not commuting at different times if we work with small enough $\epsilon$. Therefore, we may differentiate any one factor of this product by using the standard

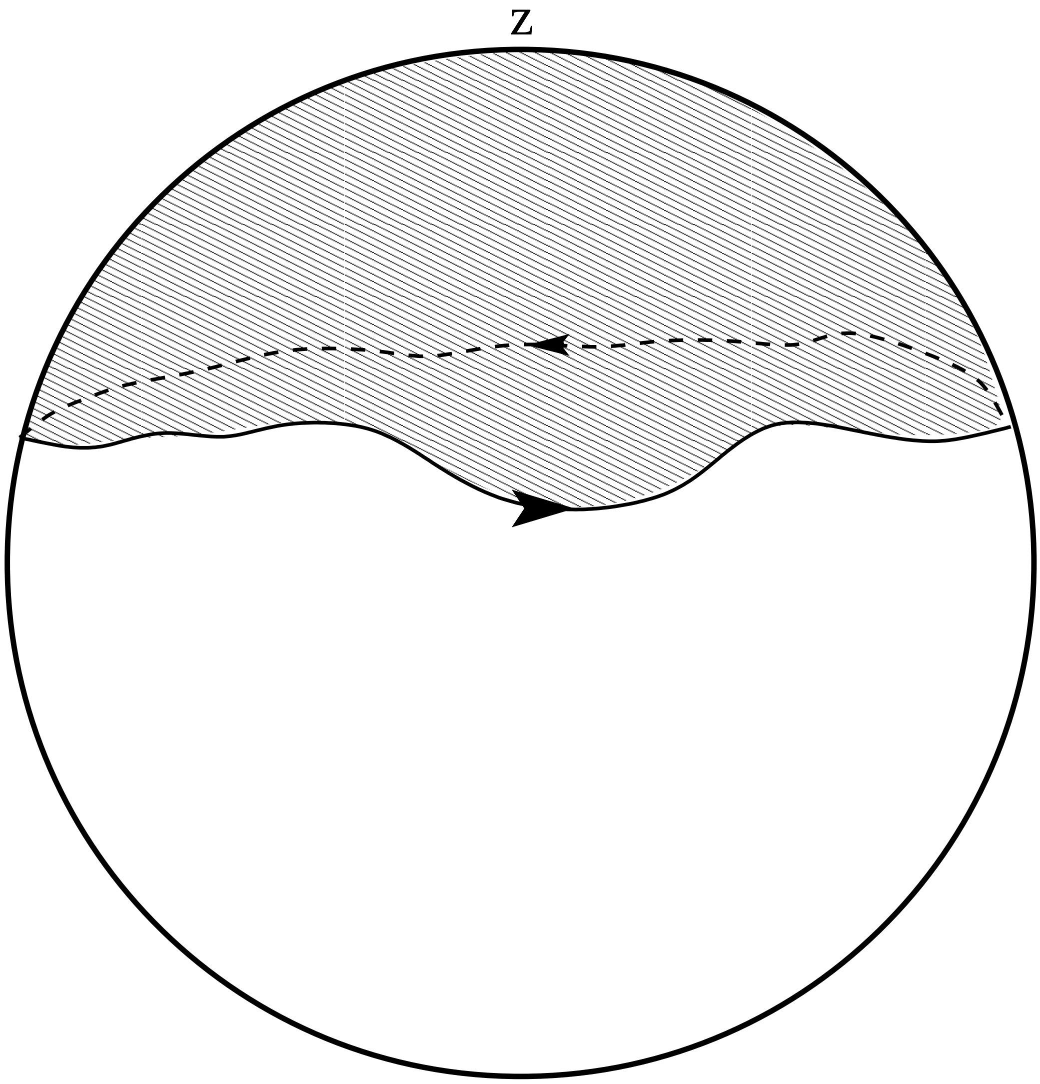


Figure 1: Closed path inscribed on unit sphere by unit vector $\vec{N(\tau)}$. Area $\mathcal{A}_z$ of spherical cap swept by this trajectory (the subscript $z$ reminds us to choose the cap that includes the North Pole) is precisely the quantity that enters the expression for the Berry phase associated with this path.

chain rule. Further, since the product rule of differentiation generalizes in an obvious way to a product of operators, we thus obtain

$$\frac{d}{d\tau}\exp(O(\tau)) \;=\; \sum_{k=0}^{M-1} \underbrace{e^{\epsilon O(\tau)} \ldots e^{\epsilon O(\tau)}}_{M-k} \frac{dO(\tau)}{d\tau} \underbrace{e^{\epsilon O(\tau)} \ldots e^{\epsilon O(\tau)}}_{k} \quad \text{with} \quad M\epsilon = 1 \tag{9}$$

Clearly, this becomes more and more accurate in the limit of $\epsilon \to 0$, $M \to \infty$, with $M\epsilon$ fixed equal to 1.

In this "continuum" limit, our formula clearly reduces to

$$\frac{d}{d\tau}e^{O(\tau)} = \int_0^1 du \exp\left((1-u)O(\tau)\right) \frac{dO(\tau)}{d\tau} \exp\left(uO(\tau)\right) \tag{10}$$

Now that we have obtained by heuristic means a formula that generalizes the chain rule to our operator-valued case, it is of course possible to *check* its validity in a perfectly rigorous way by expanding all exponentials in a power series, and comparing coefficients of

$$(O(\tau))^m \frac{dO(\tau)}{d\tau}(O(\tau))^{m'} \tag{11}$$

for $m, m' \geq 0$ on both sides of the claimed formula. This reduces to checking that

$$\int_0^1 du \frac{(1-u)^{n-k-1}u^k}{(n-k-1)!\,k!} \;=\; \frac{1}{n!} \quad \text{for} \quad k = 0\,,\,1\ldots n-1 \quad \& \quad \text{all integer} \quad n > 0 \tag{12}$$

And this is easy to check by doing the integral on the left hand side by repeated integration by parts.

We now use this to obtain a more explicit formula for $S_B$. To do this, we start by computing the overlap of $|\vec{N}(\tau)\rangle$ with its derivative:

$$\langle \vec{N}(\tau)|\frac{d}{d\tau}\vec{N}(\tau)\rangle \;=\;$$

$$\int_0^1 du \langle \psi_z | e^{+iu\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}} \left(-i\frac{d}{d\tau}[\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}]\right) e^{-iu\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}}|\psi_z\rangle$$

$$= \int_0^1 du \langle \vec{N}(u,\tau)| \left(-i\frac{d}{d\tau}[\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\vec{S}]\right) |\vec{N}(u,\tau)\rangle$$

$$= \quad -iS\int_0^1 du\vec{N}(u,\tau)\cdot\left[\vec{M}(\vec{N}(\tau))\frac{d\theta(\vec{N}(\tau))}{d\tau}+\theta(\vec{N}(\tau))\frac{d\vec{M}(\vec{N}(\tau))}{d\tau}\right] \tag{13}$$

In the above, $\vec{N}(u,\tau)$ corresponds to the direction obtained by rotating $\hat{z}$ by $u\theta(\vec{N}(\tau))$ about the axis $\vec{M}(\vec{N}(\tau))$ instead of the full angle $\theta(\vec{N}(\tau))$. Now, we note that

$$\vec{M}(\vec{N}(\tau))\cdot\vec{N}(u,\tau) \quad = \quad 0 \quad \forall u \tag{14}$$

and use this to obtain the simpler expression

$$\begin{aligned} \langle\vec{N}(\tau)|\frac{d}{d\tau}\vec{N}(\tau)\rangle &= \\ &= -iS\theta(\vec{N}(\tau))\int_0^1 du\vec{N}(u,\tau)\cdot\frac{d\vec{M}(\vec{N}(\tau))}{d\tau} \end{aligned} \tag{15}$$

Now, this allows us to write $S_B$ as

$$S_B \quad = \quad -iS\int_0^\beta d\tau\theta(\vec{N}(\tau))\int_0^1 du\vec{N}(u,\tau)\cdot\frac{d\vec{M}(\vec{N}(\tau))}{d\tau} \tag{16}$$

Integrating by parts with respect to $\tau$ gives us the alternate form

$$S_B \quad = \quad +iS\int_0^\beta d\tau\int_0^1 du\,\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau))\cdot\frac{\partial\vec{N}(u,\tau)}{\partial\tau} \tag{17}$$

Now, we note the geometric identity

$$\theta(\vec{N}(\tau))\vec{M}(\vec{N}(\tau)) \quad = \quad \vec{N}(u,\tau)\times\frac{\partial\vec{N}(u,\tau)}{\partial u} \tag{18}$$

valid for all $u\in[0,1]$ [this is easy to check by separately checking that the magnitude and direction both match]. This allows us to finally write

$$\begin{aligned} S_B &= +iS\int_0^\beta d\tau\int_0^1 du\,(\vec{N}(u,\tau)\times\frac{\partial\vec{N}(u,\tau)}{\partial u})\cdot\frac{\partial\vec{N}(u,\tau)}{\partial\tau} \\ &= +iS\int_0^\beta d\tau\int_0^1 du\,\vec{N}(u,\tau)\cdot(\frac{\partial\vec{N}(u,\tau)}{\partial u}\times\frac{\partial\vec{N}(u,\tau)}{\partial\tau}) \end{aligned} \tag{19}$$

Now, this has a very nice and obvious geometric interpretation, as being $iS$ times the (oriented) area $\mathcal{A}_z$ of the spherical cap swept out by the periodic path $\vec{N}(\tau)$ (with the subscript $z$ emphasizing that we should choose the cap that encloses the North Pole). This is shown in the accompanying figure (Fig. 1), and is the simplest and most intuitive characterization of the Berry phase factor in the weight of each path.

In later lectures, we will have more to say about the consequences of this term for quantum antiferromagnets, but for now, let me just reemphasize that this possibility of having phase factors attached to the "classical Boltzmann weight" is a general feature of the mapping between quantum statistical mechanics in $d$ dimensions and "classical statistical mechanics" in $d+1$ dimensions, and prevents us from using computational Monte-Carlo simulation methods of classical statistical mechanics for many interesting quantum systems.

In the foregoing, we had used a reference state $\psi_z$ to rotate into $|\vec{N}\rangle$ starting from the North Pole. If instead, we had used $\psi_{-z}$ to rotate into $|\vec{N}\rangle$ starting from the South Pole, then we would have got $S'_B = iS\mathcal{A}_{-z}$. Would this cause an ambiguity in the actual phase factor attached to each path? To address this, note that $S_B - S'_B = iS(\mathcal{A}_z - \mathcal{A}_{-z}) = \pm 4\pi i S$, since $\mathcal{A}_z - \mathcal{A}_{-z} = \pm 4\pi$, the area of the unit sphere. So the two conventions would differ by $\pm 4\pi i S$ in the exponential.

Since $S$ is always half-integer, this causes no ambiguity in the phase factor associated with a path, as it should not. This is perhaps the world's most complicated way of seeing that spin angular momentum must be quantized to half-integer values (in units of $\hbar$)!

In any case, let us wrap up this lecture by displaying the full expression for the coherent state path integral formulation of the partition function of the Heisenberg antiferromagnet:

$$
\begin{aligned}
Z &= \\
&\int \mathcal{D}\vec{N}(\vec{r}_i,\tau)\exp(\int_0^\beta d\tau[\sum_i +iS\int_0^1 du\,\vec{N}(\vec{r}_i,u,\tau)\cdot(\frac{\partial\vec{N}(\vec{r}_i,u,\tau)}{\partial u}\times\frac{\partial\vec{N}(\vec{r}_i,u,\tau)}{\partial\tau}) \\
&\qquad -JS^2\sum_{\langle i,j\rangle}\vec{N}(\vec{r}_i,\tau)\cdot\vec{N}(\vec{r}_j,\tau)]) \\
&\qquad \text{with constraint } \vec{N}(\vec{r}_i,0) = \vec{N}(\vec{r}_i,\beta)\ \ \forall i \qquad (20)
\end{aligned}
$$