Lecture 8: Path integral for spin systems

In the last lecture, we constructed the overcomplete basis of spin coherent states and worked out the correct form of the resolution of identity and representation of spin operators in this basis.

Now, we use this to develop the coherent state path integral for the quantum statistical mechanics of spin systems. The first step is to note that

$$\text{Tr}(A) = (2S+1) \int \frac{d\vec{N}}{4\pi} \langle \vec{N}|A|\vec{N} \rangle \tag{1}$$

for any operator A. This is actually a simple consequence of the resolution of identity

$$\mathbb{1} = (2S+1) \int \frac{d\vec{N}}{4\pi} |\vec{N} \rangle \langle \vec{N}| \tag{2}$$

derived in the previous lecture. To see this, simply start with any orthonormal basis

$$\{|\alpha\rangle\} \tag{3}$$

and use the resolution of identity in the coherent state basis to argue as follows:

$$
\begin{aligned}
\text{Tr}(A) &\equiv \sum_\alpha \langle \alpha|A|\alpha \rangle \\
&= \sum_\alpha (2S+1) \int \frac{d\vec{N}}{4\pi} \langle \alpha|\vec{N} \rangle \langle \vec{N}|A|\alpha \rangle \\
&= (2S+1) \int \frac{d\vec{N}}{4\pi} \sum_\alpha \langle \vec{N}|A|\alpha \rangle \langle \alpha|\vec{N} \rangle \\
&= (2S+1) \int \frac{d\vec{N}}{4\pi} \langle \vec{N}|A|\vec{N} \rangle \tag{4}
\end{aligned}
$$

We are now in a position to use this coherent state basis to construct the spin path integral by following the strategy we outlined in the previous lecture. To see how this goes more clearly, let us begin by considering a single spin in a magnetic field, *i.e.* a Hamiltonian

$$H(\vec{S}) = -\vec{B} \cdot \vec{S} \tag{5}$$

For this simple case, we write

$$
\begin{aligned}
\mathrm{Tr}(e^{-\beta H(\vec{S})}) &= \frac{2S+1}{4\pi} \int d\vec{N}_0 \langle \vec{N}_0 | e^{-\beta H(\vec{S})} | \vec{N}_0 \rangle \\
&= \left(\frac{2S+1}{4\pi}\right)^M \int d\vec{N}_0 \int d\vec{N}_\epsilon \cdots \int d\vec{N}_{(M-1)\epsilon} \prod_{k=0}^{M-1} \langle \vec{N}_{(k+1)\epsilon} | e^{-\epsilon H} | \vec{N}_{k\epsilon} \rangle \\
&\text{with } |\vec{N}_{M\epsilon}\rangle \equiv |\vec{N}_0\rangle \text{ and } M\epsilon = \beta
\end{aligned}
\tag{6}
$$

We now take the limit of large M, so that the corresponding ϵ is small, and ask: For small enough ϵ, can we write

$$
\langle N(\tau+\epsilon) | e^{-\epsilon H(\vec{S})} | N(\tau) \rangle
\tag{7}
$$

as the exponential of something tractable? If the answer is yes, then we are "in business", and we can go ahead and derive a "nice" path integral representation of the partition function.

Let's explore this question by expanding

$$
\langle N(\tau+\epsilon) | e^{-\epsilon H(\vec{S})} | N(\tau) \rangle
\tag{8}
$$

to linear order in ϵ. To do this, we note that there are two sources of linear terms in ϵ, namely the ϵ dependence of the bra, and the ϵ dependence of $\exp(-\epsilon H(\vec{S}))$. Putting these together, we obtain

$$
\langle N(\tau+\epsilon) | e^{-\epsilon H(\vec{S})} | N(\tau) \rangle = 1 - \epsilon \left(\langle N(\tau) | \frac{d}{d\tau} N(\tau) \rangle + H(S\vec{N}(\tau)) \right) + \ldots
\tag{9}
$$

In obtaining the second term of the above equation, we have used the fact that the single-spin Hamiltonian is a *linear* function of the spin operator, and its expectation value in a state $|\vec{N}(\tau)\rangle$ can therefore be calculated simply by replacing (in $H(\vec{S})$) the operator $\vec{S}$ with the vector $S\vec{N}(\tau)$. Of course, if we were dealing with spin $S = 1/2$, this would not be a restrictive assumption, since the square of a spin-half operator is anyway proportional to the identity operator, and therefore the most general single-spin Hamiltonian for a spin-half moment is always a linear function of the spin operator. However, it is important to keep this restriction in mind when working with spin $S >$

1/2 systems. For more general Hamiltonians in the spin $S > 1/2$ cases, the expectation value of $H(\vec{S})$ in state $|\vec{N}(\tau)\rangle$ can still be represented as a function of $\vec{N}(\tau)$, but the function is not simply $H(S\vec{N}(\tau))$. Before we proceed further with the derivation of the path integral, a small aside on this question is perhaps necessary to clarify this point: Consider for instance a single-spin Hamiltonian of the form $H_{zz} = S_z^2$, for a spin $S > 1/2$ moment. Such *a single-ion anisotropy term* in the Hamiltonian represents the effects of the coupling of spin and orbital degrees of freedom of a magnetic ion via spin-orbit interactions familiar from atomic physics. To compute the expectation value of such a term in the state $|\vec{N}(\tau)\rangle$, we need to take recourse to the integral representation of the spin operator, which we mentioned without proof in the previous lecture:

$$\vec{S} = (S+1)(2S+1) \int \frac{d\vec{N}_1}{4\pi} \vec{N}_1 |\vec{N}_1\rangle\langle\vec{N}_1| \tag{10}$$

From this, we can deduce the following representation of S_z^2:

$$S_z^2 = (S+1)^2(2S+1)^2 \int\int \frac{d\vec{N}_1}{4\pi}\frac{d\vec{N}_2}{4\pi} N_1^z N_2^z |\vec{N}_1\rangle\langle\vec{N}_1|\vec{N}_2\rangle\langle\vec{N}_2| \tag{11}$$

Using this, we can write

$$\langle\vec{N}(\tau)|S_z^2|\vec{N}(\tau)\rangle = (S+1)^2(2S+1)^2 \int\int \frac{d\vec{N}_1}{4\pi}\frac{d\vec{N}_2}{4\pi} N_1^z N_2^z \langle\vec{N}(\tau)|\vec{N}_1\rangle\langle\vec{N}_1|\vec{N}_2\rangle\langle\vec{N}_2|\vec{N}(\tau)\rangle \tag{12}$$

which defines a somewhat complicated function of S and $\vec{N}(\tau)$ but poses no conceptual difficulty in the proceeding further with our derivation of the path integral.

With this out of the way, we proceed further by observing that we can equally well write

$$1 - \epsilon\left(\langle N(\tau)|\frac{d}{d\tau}N(\tau)\rangle + H(S\vec{N}(\tau))\right) + \ldots \tag{13}$$

as

$$\exp\left[-\epsilon\left(\langle N(\tau)|\frac{d}{d\tau}N(\tau)\rangle + H(S\vec{N}(\tau))\right)\right]$$

(14)

to linear order in ϵ, and therefore we have the approximate equality

$$\langle N(\tau+\epsilon)|e^{-\epsilon H(\vec{S})}|N(\tau)\rangle \approx \exp\left[-\epsilon\left(\langle N(\tau)|\frac{d}{d\tau}N(\tau)\rangle + H(S\vec{N}(\tau))\right)\right]$$

(15)

Thus, we have the following representation of the partition function

$$Z = \text{Tr}(e^{-\beta H(\vec{S})}) =$$
$$\left(\frac{2S+1}{4\pi}\right)^M \int d\vec{N}_0 \int d\vec{N}_\epsilon \cdots \int d\vec{N}_{(M-1)\epsilon} \prod_{k=0}^{M-1} \exp\left[-\epsilon\left(\langle N(\tau_k)|\frac{d}{d\tau_k}N(\tau_k)\rangle + H(S\vec{N}(\tau_k))\right)\right]$$
$$\text{with} \quad \tau_k = k\epsilon$$

(16)

In the limit $M \to \infty$ and $\epsilon \to 0$, keeping $M\epsilon$ fixed equal to β, this *defines* the path integral representation of the partition function, and we write

$$Z = \int_{\vec{N}(\beta)=\vec{N}(0)} \mathcal{D}\vec{N}(\tau) \exp\left(-\int_0^\beta d\tau\left[\langle\vec{N}(\tau)|\frac{d}{d\tau}\vec{N}(\tau)\rangle + H(S\vec{N}(\tau))\right]\right)$$

(17)

with the understanding that $H(S\vec{N}(\tau))$ is to be replaced by a more complicated function of S and $\vec{N}(\tau)$ if the Hamiltonian is not linear in the spin operator $\vec{S}$.

This completes our derivation of the coherent state path integral for a single spin. What about generalizations to more realistic d dimensional system made up of L^d spins interacting with each other via some couplings? While this may seem to involve a big additional step in terms of complexity, in actual fact we have already done all the hard work, and the generalization is rather straightforward, at least for a large class of useful and realistic Hamiltonians. To see this, we consider any "multilinear" Hamiltonian

$H(\vec{S}_1, \vec{S}_2, \ldots \vec{S}_{L^d})$ which is *linear when considered a function of any individual* $\vec{S}_i$. For any such Hamiltonian, the procedure outlined in the foregoing derivation goes through essentially unchanged. This is because we can work with multi-spin coherent states $|\vec{N}_1, \vec{N}_2 \ldots \vec{N}_{L^d}\rangle$ constructed analogously to the single-spin case:

$$
|\vec{N}_1, \vec{N}_2 \ldots \vec{N}_{L^d}\rangle =
$$
$$
\exp(-i\theta_1 \vec{M}_1 \cdot \vec{S}_1 - i\theta_2 \vec{M}_2 \cdot \vec{S}_2 \ldots - i\theta_{L^d} \vec{M}_{L^d} \cdot \vec{S}_{L^d}) \ |\hat{z}\rangle_1 |\hat{z}\rangle_2 \ldots |\hat{z}\rangle_{L^d}
$$
$$
\text{where} \ \ \theta_i \ = \ \theta(\vec{N}_i) \ , \ \ \vec{M}_i \ = \ \vec{M}(\vec{N}_i)
$$

(18)

Now, since the expectation value of any "multilinear" Hamiltonian $H(\vec{S}_1, \vec{S}_2, \ldots \vec{S}_{L^d})$ in a coherent state $|\vec{N}_1(\tau), \vec{N}_2(\tau) \ldots \vec{N}_{L^d}(\tau)\rangle$ can be written as

$$
\langle \vec{N}_1(\tau), \vec{N}_2(\tau) \ldots \vec{N}_{L^d}(\tau)|H(\vec{S}_1, \vec{S}_2, \ldots \vec{S}_{L^d})|\vec{N}_1(\tau), \vec{N}_2(\tau) \ldots \vec{N}_{L^d}(\tau)\rangle \ =
$$
$$
H(S\vec{N}_1(\tau), S\vec{N}_2(\tau) \ldots S\vec{N}_{L^d}(\tau))
$$

(19)

the foregoing single-spin derivation goes throught without any real change. Thus, for the case of a d dimensional "Heisenberg Antiferromagnet" with Hamiltonian

$$
H \ = \ J \sum_{\langle ij \rangle} \vec{S}(\vec{r}_i) \cdot \vec{S}(\vec{r}_j)
$$

(20)

where $\langle ij \rangle$ denote nearest neighbour bonds of the d dimensional lattice and $\vec{r}_i$ are the lattice positions, we have

$$
Z \ =
$$
$$
\int \mathcal{D}\vec{N}(\vec{r}_i, \tau) \exp\left(-\int_0^\beta d\tau \left[\sum_i \langle \vec{N}(\vec{r}_i, \tau)|\frac{d}{d\tau}\vec{N}(\vec{r}_i, \tau)\rangle + JS^2 \sum_{\langle i,j \rangle} \vec{N}(\vec{r}_i, \tau) \cdot \vec{N}(\vec{r}_j, \tau)\right]\right)
$$
$$
\text{with constraint} \ \ \vec{N}(\vec{r}_i, 0) \ = \ \vec{N}(\vec{r}_i, \beta) \ \ \forall i
$$

(21)

Again, the generalization to Hamiltonians which are not separately linear in each spin operator $\vec{S}(\vec{r}_i)$, for instance due to the presence of single-ion

anisotropy terms, is conceptually straightforward, and involves replacing $H(S\vec{N}(\vec{r}_i, \tau))$ by a more complicated function of S and the $\vec{N}(\vec{r}_i, \tau)$.

We conclude this lecture with one final observation: If it were not for the first term involving the overlap of $|\vec{N}(\tau)\rangle$ with its own derivative, the weight of a path would have been precisely the classical Boltzmann weight of a classical model of unit-vectors $\vec{N}$ interacting with a classical exchange energy JS^2. This is a major advantage of the present path integral representation, since this means that the classical energy of a configuration of the $\{\vec{N}(\vec{r}_i)\}$ plays an important role in determining which paths dominate the path integral representation of the quantum problem, and this allows us to bring to bear all our intuition about the behaviour of the classical system to learn something about the corresponding quantum problem.

Of course, it is still true that the first term contains all the important information about the quantum dynamics of the system, and clearly, we need to come to grips with this term to fully understand the behaviour of a *quantum* antiferromagnet—this is precisely what we will focus on in the next lecture.