Lecture 7: Path integral representation and spin coherent states

In the first five lectures of this course, we have seen how Statistical Mechanics provides a prescription for the calculation of macroscopic properties of many-particle systems, and understood that this prescription is not something that can be applied automatically "by rote"—indeed, we have seen that it involves introducing new ideas and concepts at each step to account for the emergent properties of such macroscopic systems. We have also seen how experimental measurements can be modeled by linear response theory, which relates the response of the system to certain correlation functions of the equilibrium system.

At this point, we need to ask: Is there a convenient formalism or language in which one can calculate these correlation functions, or at least develop some intuition for, or qualitative understanding of, these correlation functions? The answer turns out to be the idea that $\mathrm{Tr}\exp(-\beta H)$ for a d dimensional quantum system at inverse temperature $\beta \equiv (k_B T)^{-1}$ can be represented as a sum over "paths" in a $d+1$ dimensional space-"time" in which the "time" direction is along the imaginary axis, and is of finite extent equal to β. Provided the weight of each path in this sum over paths is real and positive, this is equivalent to mapping the quantum statistical mechanics of the original d dimensional system to the *classical statistical mechanics* of a classical system in $d+1$ dimensions, of which one dimension has finite extent. We will see later in this course that there are interesting situations in which the weight over paths is not real and positive, due to the presence of quantum mechanical "Berry phases" in the weight. In these cases, the path integral approach is difficult to use as a calculational prescription. Nevertheless, it continues to provide insights that are not easily obtained by other means.

With this background, consider then

$$
\begin{aligned}
Z &= \mathrm{Tr} e^{-\beta H} = \mathrm{Tr}\, \underbrace{e^{-\epsilon H} \; e^{-\epsilon H}}_{M} \quad \text{with} \quad M\epsilon = \beta \\
&= \sum_{\alpha_0, \alpha_\epsilon, \alpha_{2\epsilon} \cdots \alpha_{(M-1)\epsilon}} \prod_{k=0}^{M-1} \langle \alpha_{(k+1)\epsilon} | e^{-\epsilon H} | \alpha_{k\epsilon} \rangle \quad \text{with} \quad |\alpha_{M\epsilon}\rangle \equiv |\alpha_0\rangle
\end{aligned}
\tag{1}
$$

In the above, we have simply written $\exp(-\beta H)$ as a product of M identical factors $\exp(-\epsilon H)$ with $\epsilon \equiv \beta/M$, and then introduced the following resolution of identity

$$\sum_{\alpha} |\alpha\rangle\langle\alpha| \quad = \quad \mathbb{1} \tag{2}$$

between each successive factor in this product. Here, $\{|\alpha\rangle\}$ are a complete set of orthonormal states that form a basis. Now, if we could write

$$\langle\alpha_{k+1}|e^{-\epsilon H}|\alpha_k\rangle \quad = \quad \exp[-\epsilon S(\alpha_{k\epsilon})] \; , \tag{3}$$

with S a "nice" function, then, we would obtain the following representation of the partition function

$$Z \quad = \sum_{\alpha_0,\alpha_\epsilon,\cdots,\alpha_{(M-1)\epsilon}} \exp\left[-\epsilon \sum_{k=0}^{M-1} S(\alpha_{k\epsilon})\right] \tag{4}$$

This has the following nice interpretation: Think of the system evolving in imaginary time τ—*i.e.* under the action of the evolution operator $\exp(-H\tau)$ instead of $\exp(-iHt)$— from the initial state $|\alpha_0\rangle$ at the "initial time" $\tau = 0$ along a closed path in α space, back to state $|\alpha_0\rangle$ at the "final time" $\tau = \beta$. The sequence of states

$$\{|\alpha_0\rangle, |\alpha_\epsilon\rangle, \cdots, |\alpha_{(M-1)\epsilon}\rangle\}$$

represents a "stroboscopic" sampling of this path in α space at the discrete sequence of "times"

$$\{0, \epsilon, \cdots, (M-1)\epsilon\} \; .$$

The corresponding weight of this closed path is

$$\exp\left(-\epsilon \sum_{k=0}^{M-1} S(\alpha_{k\epsilon})\right) \tag{5}$$

which may also be written as

$$\exp\left(-\int_0^\beta d\tau S(\alpha(\tau))\right) \text{ in limit } M \to \infty, \epsilon \to 0, M\epsilon = \beta \text{ constant,} \tag{6}$$

i.e. in the limit of "infinitely fast sampling" of the imaginary time evolution. In practice, this limit of infinitely fast sampling is a useful conceptual device, because we can usually write

$$\langle \alpha_{k+1} | e^{-\epsilon H} | \alpha_k \rangle \quad = \quad \exp[-\epsilon S(\alpha_{k\epsilon})] \tag{7}$$

(with S a nice calculable function) only in the limit of infinitely small ϵ.

In this limit, the multiple summation

$$\sum_{\alpha_0, \alpha_\epsilon, \cdots, \alpha_{(M-\epsilon)}} \tag{8}$$

is like an "integral" over all possible periodic paths in the "space of paths'. We can schematically write this as

$$\int_{\alpha(0)=\alpha(\beta)} \mathcal{D}\alpha(\tau) \; , \tag{9}$$

to finally obtain the *path integral representation of the partition function*:

$$Z \quad = \quad \int_{\alpha(0)=\alpha(\beta)} \mathcal{D}\alpha(\tau) \exp\left(- \int_0^\beta d\tau S[\alpha(\tau)] \right) \tag{10}$$

If the *action functional* S is real and positive, then we have in effect mapped the quantum statistical mechanics of the d dimensional quantum system to the *classical statistical mechanics* of an equivalent classical system that lives in $d+1$ dimensions—the extra imaginary time dimension is continuous in nature, and finite in extent, while the d spatial dimensions of the original system remain unchanged in character and extent.

This is clearly a very attractive reformulation, but the real question becomes: What set $|\alpha\rangle$ do we use for a particular system? In the rest of this lecture, and in the next few lectures, we will address this question in turn for quantum spin systems, quantum systems of bosonic particles, and quantum systems of fermionic particles. These examples will serve to fix the foregoing formal developments firmly in our minds, and will be useful starting points for a further study of the statistical mechanics of these systems.

In the remainder of this lecture, we define a particularly convenient albeit over-complete and non-orthogonal basis made up of the *spin coherent states*, and demonstrate that they provide a very natural and useful basis for developing a path integral representation of quantum spin systems. In particular, we will explicitly see that the over-complete and non-orthogonal nature of this basis poses no serious difficulty in the implementation of the foregoing strategy to rewrite the partition function as a functional integral.

We begin by considering a single spin-half moment, which has a two dimensional Hilbert space spanned by the two states

$$\{|\uparrow\rangle, |\downarrow\rangle\} \tag{11}$$

in which the spin is quantized along z axis to have z projection $\pm 1/2$. In standard linear algebra notation, we may represent these two basis vectors of this two dimensional space as

$$|\uparrow\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{12}$$

For a d dimensional system which has a spin-half variable on each of L^d sites, the Hilbert space is a product of such independent two-dimensional spaces, and has total dimension equal to $2^{(L^d)}$. An obvious orthonormal basis is the set

$$\{|\sigma_1 \sigma_2 \cdots \sigma_{L^d}\rangle\} \tag{13}$$

where each σ can be $\uparrow$ or $\downarrow$. However, this is not at all convenient, when it comes to developing a path integral representation, since the basis is made up of discrete possibilities for the σ and it is hard to develop any intuition for "paths" in this space.

A much more convenient basis is the basis of spin coherent states $\{|\vec{N}\rangle\}$, which we first define for a single spin-half variable by writing

$$|\vec{N}\rangle = |m_{\vec{N}} = \frac{1}{2}\rangle \; . \tag{14}$$

In other words $|\vec{N}\rangle$ is the $m_{\vec{N}} = \frac{1}{2}$ state which is fully polarized along the quantization axis (unit vector) $\vec{N}$.

More explicitly, when

$$\vec{N} = \hat{z} = (0,0,1) \tag{15}$$

we have

$$|\vec{N} = \hat{z}\rangle \equiv |\uparrow\rangle \tag{16}$$

and all other states $|\vec{N}\rangle$ can be obtained from this reference state

$$|\vec{N} = \hat{z}\rangle \equiv |\psi_z\rangle \equiv |\uparrow\rangle \tag{17}$$

by applying an appropriate rotation operator in spin-space. To do this, we recall that if we are given a state $|\psi\rangle$, and we want to obtain from it the rotated state $|R\psi\rangle$, where R denotes a rotation with rotation angle θ about axis (unit vector) $\vec{A}$, then we may write

$$|R\psi\rangle \quad = \quad e^{+i\theta\vec{L}\cdot\vec{A}}|\psi\rangle \tag{18}$$

where $\vec{L}$ is total angular momentum operator appropriate to the system—in the case of a single spin, this is clearly

$$\vec{L} \quad = \quad \vec{S} \tag{19}$$

where $\vec{S}$ is the spin operator, while for a system consisting of many spins, it is

$$\vec{L} \quad = \quad \vec{S}_{\text{tot}} \tag{20}$$

where $\vec{S}_{\text{tot}}$ is the total spin operator (*i.e.* the sum of the individual spin operators taken over all the magnetic moments in the system).

What constitutes a convenient choice of axis (unit vector) $\vec{A}$ and angle θ to obtain $|\vec{N}\rangle$ from the reference state $|\psi_z\rangle$? It turns out that the answer is the following: Draw the projection of the unit vector $\vec{N}$ onto the xy plane. If

$$\vec{N} \quad = \quad (\sin(\theta)\cos(\phi)\ ,\ \sin(\theta)\sin(\phi)\ ,\ \cos(\theta)) \tag{21}$$

this projection makes an angle of ϕ with the x axis and has length $\sin(\theta)$. Now, draw a unit vector $\vec{M}$ in the xy plane, so that it is perpendicular to this projection, and makes a *right handed triad* with $\hat{z}$ and this projection of $\vec{N}$ onto the xy plane. This uniquely specifies $\vec{M}$ to be

$$\vec{M} \quad = \quad (\cos(\phi+\pi/2)\ ,\ \sin(\phi+\pi/2)\ ,\ 0) \tag{22}$$

Then, $|\vec{N}\rangle$ can be obtained from $|\psi_z\rangle$ by rotating about the axis $\vec{M}$ by an angle of $-\theta$:

$$|\vec{N}\rangle \quad = \quad e^{-i\theta\vec{M}\cdot\vec{S}}|\psi_z\rangle \tag{23}$$

Our over-complete basis is thus

$$\{\exp(-i\theta(\vec{N})\vec{M}(\vec{N})\cdot\vec{S})|\psi_z\rangle\} \tag{24}$$

where $\vec{N}$ ranges over the unit-sphere in three dimensions.

This basis is "very" over-complete, in the sense that

$$\langle\vec{N}_1|\vec{N}_2\rangle \neq 0 \tag{25}$$

for any pair of unit vectors $\vec{N}_1$ and $\vec{N}_2$ unless $\vec{N}_1 = -\vec{N}_2$. Indeed, it turns out that

$$|\langle N_1|N_2\rangle|^2 = \frac{1+\vec{N}_1\cdot\vec{N}_2}{2}\ . \tag{26}$$

How do we go about checking something like this? The simplest way is to construct the states $|\vec{N}\rangle$ *explicitly*. To do this, we recall that

$$S_x = \frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \equiv \frac{\sigma_x}{2},\ S_y = \frac{1}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \equiv \frac{\sigma_y}{2},\ S_z = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \equiv \frac{\sigma_z}{2} \tag{27}$$

Also, we recall

$$\begin{aligned}\sigma_x^2 &= \sigma_y^2 = \sigma_z^2 = 1 \ \text{ and}\\ \sigma_x\sigma_y &= i\sigma_z \ \text{ and cyclic permutations.}\end{aligned} \tag{28}$$

Next, we expand the rotation operator in a power series in θ

$$e^{-i\theta\vec{M}\cdot\vec{S}} = 1\!\!1 + (-i\theta)\vec{M}\cdot\vec{S} + \frac{(-i\theta)^2}{2!}(\vec{M}\cdot\vec{S})^2 + \cdots \tag{29}$$

and note that

$$\begin{aligned}(\vec{M}\cdot\vec{S})^2 &= 1\!\!1 + \left[\frac{m_x m_y}{4}\{\sigma_x\ ,\ \sigma_y\} + \frac{m_y m_z}{4}\{\sigma_y\ ,\ \sigma_z\} + \frac{m_z m_x}{4}\{\sigma_z\ ,\ \sigma_x\}\right]\\ &= 1\!\!1,\end{aligned} \tag{30}$$

where we have used

$$\begin{aligned}\{\sigma_\mu\ ,\ \sigma_\nu\} &\equiv \sigma_\mu\sigma_\nu + \sigma_\nu\sigma_\mu\\ &= 2\delta_{\mu,\nu}\ .\end{aligned} \tag{31}$$

So, we have

$$
\begin{aligned}
e^{-i\theta \vec{M}\cdot\vec{S}} &= \cos(\frac{\theta}{2})\mathbb{1} - i\sin(\frac{\theta}{2})\vec{M}\cdot\sigma \\
&= \cos(\frac{\theta}{2})\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - i\sin(\frac{\theta}{2})\begin{pmatrix} m_z & m_x - im_y \\ m_x + im_y & -m_z \end{pmatrix} \\
&= \begin{pmatrix} \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2})e^{-i\phi} \\ \sin(\frac{\theta}{2})e^{i\phi} & -\cos(\frac{\theta}{2}) \end{pmatrix}
\end{aligned}
\tag{32}
$$

Therefore, we have

$$
|\vec{N}\rangle \equiv e^{-i\theta\vec{M}\cdot\vec{S}}|\uparrow\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{+i\phi}|\downarrow\rangle \tag{33}
$$

The formula for the overlap square of two coherent states can now be proved by straightforward manipulation of trignometric identities, and you should check this for yourself.

To use this basis of coherent states for obtaining a path integral representation for quantum spin systems, two other properties are crucial. The first is the following resolution of identity in our coherent state basis:

$$
\mathbb{1} = \int \frac{d\vec{N}}{2\pi}|\vec{N}\rangle\langle\vec{N}| \tag{34}
$$

where $\int d\vec{N}$ denotes an integral over the unit sphere with the usual measure

$$
\int d\vec{N} \equiv \int_{-1}^{1} d\cos(\theta)\int_{0}^{2\pi} d\phi \tag{35}
$$

The validity of this resolution of identity is also easy to check using the explicit representation we have derived for $|\vec{N}\rangle$, and we will do so below as an illustration.

We start with

$$
\int \frac{d\phi d\cos\theta}{2\pi}\left[\cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{+i\phi}|\downarrow\rangle\right]\left[\cos\frac{\theta}{2}\langle\uparrow| + \sin\frac{\theta}{2}e^{-i\phi}\langle\downarrow|\right] \tag{36}
$$

and note that the ϕ integral eliminates the cross terms to reduce this to

$$
\int_{-1}^{1} d\cos\theta\left[\cos^2\frac{\theta}{2}|\uparrow\rangle\langle\uparrow| + \sin^2\frac{\theta}{2}|\downarrow\rangle\langle\downarrow|\right] = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| = \mathbb{1} \tag{37}
$$

The second important property, from the point of view of path integral representations, is the particularly simple form of the expectation value of the spin operator in state $|\vec{N}\rangle$:

$$\langle\vec{N}|\vec{S}|\vec{N}\rangle = \frac{\vec{N}}{2} \tag{38}$$

Finally, another interesting identity (which we will not have occasion to use explicitly in this lecture course) is the integral representation of the spin operator:

$$\vec{S} = \frac{3}{2}\int \frac{d\vec{N}}{2\pi}\vec{N}|\vec{N}\rangle\langle\vec{N}| \tag{39}$$

In the next lecture, we will use this basis and these properties to develop a coherent state path integral representation for quantum spin systems. Here, we conclude by re-emphasizing the fact that our construction of the coherent state basis is valid for any spin-S representation of $SU(2)$, although in our subsequent discussion of the properties of the basis states, we focused on the special case of $S = 1/2$ for concreteness. To emphasize this point, we list the corresponding definitions and properties for general spin S without proof:

$$\begin{aligned} |\vec{N}\rangle &= \exp(-i\theta(\vec{N})\vec{M}(\vec{N})\cdot\vec{S})|\psi_z\rangle \\ &\text{where } \; |\psi_z\rangle = |S_z = S\rangle \end{aligned} \tag{40}$$

$$\mathbb{1} = (2S+1)\int \frac{d\vec{N}}{4\pi}|\vec{N}\rangle\langle\vec{N}| \tag{41}$$

$$\langle\vec{N}|\vec{S}|\vec{N}\rangle = S\vec{N} \tag{42}$$

$$|\langle\vec{N}_1|\vec{N}_2\rangle|^2 = \left(\frac{1+\vec{N}_1\cdot\vec{N}_2}{2}\right)^{2S} . \tag{43}$$

$$\vec{S} = (S+1)(2S+1)\int \frac{d\vec{N}}{4\pi}\vec{N}|\vec{N}\rangle\langle\vec{N}| \tag{44}$$