Lecture 11

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1 Path integral for spin

We started our course by discussing the minimal quantum system, that of a spin 1/2. We found that this example is the one that best captures the formalism of kets and operators without all the complications of the continuous coordinates and infinite dimensional Hilbert spaces. For the path integral, on the other hand, we face the opposite problem. Since the formulation is rooted in continuous classical trajectories, we anticipate that the description of spin will be more subtle. In other words, since the spin 1/2 problem is the most quantum mechanical system, it is the hardest one to come up with a classical analog for. This is one of the reasons why it took a long time between the initial development of path integrals in the late 40s to the final development of the path integral for spins in the 80s. With hindsight, there is nothing really complicated about the path integral for spins, just a novel conceptual ingredient that ensures the pecularities of the finite dimensional Hilbert space is accounted for.

For definiteness, let us consider the Hamiltonian

$$\mathcal{H} = \gamma \boldsymbol{B} \cdot \boldsymbol{S} \tag{1}$$

where γ is the gyromagnetic ratio $\gamma = \frac{|e|}{ms}$ and we are assuming a particle with charge $-e$. How will we go about formulating a path integral to this problem? Let us retrace our derivation from the previous lectures. We start by writing the propagator $\langle \hat{n}_f, T | \hat{n}_i, 0 \rangle = \langle \hat{n}_f | e^{-\frac{i}{\hbar}\mathcal{H}T} | \hat{n}_i \rangle$ then dividing the time interval T into N intervals with width $\Delta t = T/N$. The crucial next step is the insertion of the resolution of the identity. Now our basis states $|\pm\rangle$ do provide a resolution of unity

$$\sum_{\sigma=\pm} |\sigma\rangle\langle\sigma| = \mathbb{1} \tag{2}$$

However, attempting to derive the path integral by inserting the above identity will not lead to a continuous family of classical paths. Instead, the paths will have to jump between $|+\rangle$ and $|-\rangle$ which will not yield a continuous limit when the intervals get very short. The problem arises from the fact that, to derive path integrals, we need a resolution of unity in terms of a set of states that **varies continuously in space**. For the position and momentum basis, this happened also to be the natural basis of the problem but for spin states, this is not the case. To resolve this issue, recall that we did not require that the resolution of unity used an orthonormal basis. Instead, it suffices to have a complete basis. We have seen from our discussion of coherent states that we can have complete sets of states that provide a resolution of unity without being orthogonal.

We would like to construct the most classical representation possible for spin states, which will provide us with an overcomplete basis, similar to coherent states, that we can use to derive the path integral. We have seen before that the ket for a spin 1/2 state whose spin is pointing in a general direction $\hat{n}$ is described

$$|\hat{n}\rangle = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}e^{i\phi}|-\rangle \tag{3}$$

which can describe any spin orientation. For example, if $|+\rangle$ and $|-\rangle$ describes spin polarization in the z-direction, then $\theta = 0, \pi$ describes the $|\pm z\rangle$ state, $\theta = \pi/2$, $\phi = 0, \pi$ describe $|\pm x\rangle$ and $\theta = \pi/2$,

$\phi = \pm\pi/2$ describe $|\pm y\rangle$. This state is the closest to a classical spin vector we can write and it satisfies the expected relation

$$\langle \hat{n}|\boldsymbol{S}|\hat{n}\rangle = \frac{\hbar}{2}\hat{n} \tag{4}$$

In fact, we will see now that the states (3) are overcomplete and thus provide a resolution of unit. First, it is clear that $|\hat{n}\rangle$ and $|\hat{n}'\rangle$ are generally non-orthogonal since

$$\langle \hat{n}|\hat{n}'\rangle = \left(\frac{1+\hat{n}\cdot\hat{n}'}{2}\right)^{1/2} \tag{5}$$

Second note that we can write a resolution of unity using

$$\int d\hat{n}|\hat{n}\rangle\langle\hat{n}| = \frac{1}{\pi}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta |\hat{n}\rangle\langle\hat{n}| = |+\rangle\langle+| + |-\rangle\langle-| = \mathbb{1} \tag{6}$$

We can now write the expression for the propagator with the resolution of unity inserted $N-1$ times and define $\hat{n}_0 = \hat{n}_i$ and $\hat{n}_N = \hat{n}_f$

$$\langle \hat{n}_f, T|\hat{n}_i, 0\rangle = \int \prod_{i=1}^{N-1} d\hat{n}_i \prod_{l=1}^{N} \langle \hat{n}_l|e^{-\frac{i}{\hbar}\mathcal{H}\Delta t}|\hat{n}_{l-1}\rangle \tag{7}$$

Similar to out discussion last lecture, we can simplify the time evolution over a very short time segment as

$$\begin{aligned}
\langle \hat{n}_l|e^{-\frac{i}{\hbar}\mathcal{H}\Delta t}|\hat{n}_{l-1}\rangle &= \langle \hat{n}_l|\hat{n}_{l-1}\rangle - \gamma\frac{i}{2}\Delta t\boldsymbol{B}\cdot\hat{n}\langle\hat{n}_l|\hat{n}_l\rangle \\
&= 1 + [\langle \hat{n}_l|\hat{n}_{l-1}\rangle - \langle\hat{n}_l|\hat{n}_l\rangle] - \gamma\frac{i}{2}\Delta t\boldsymbol{B}\cdot\hat{n} \\
&= 1 + \Delta t[-\langle\hat{n}_l|\partial_t\hat{n}_l\rangle - \gamma\frac{i}{2}\boldsymbol{B}\cdot\hat{n}] = e^{-\Delta t[\langle\hat{n}_l|\partial_t\hat{n}_l\rangle + \frac{i}{2}\gamma\boldsymbol{B}\cdot\hat{n}]}
\end{aligned} \tag{8}$$

Here, we have assumed that $\hat{n}$ does not change much over an infinitesmal interval Δt. Substituting in (7) gives

$$\langle \hat{n}_f, T|\hat{n}_i, 0\rangle = \int \mathcal{D}\hat{n}(t)e^{\frac{i}{\hbar}S[\hat{n}(t)]}, \qquad \mathcal{D}\hat{n}(t) = \prod_{i=1}^{N-1} d\hat{n}_i, \qquad S[\hat{n}(t)] = \hbar\int_0^T dt[i\langle n|\partial_t n\rangle - \frac{\gamma}{2}\boldsymbol{B}\cdot\hat{n}] \tag{9}$$

The second term above is the term we expect from the Hamiltonian by thinking of $\boldsymbol{B}\cdot\boldsymbol{S}$ as a potential energy. The first term is the unexpected term that crucially captures the essense of the quantum mechanical nature of the spin. It can be understood as the analog of the classical $p\dot{x}$ term that is used in the Legendre transform to construct the Lagrangian from the Hamiltonian.

Let us first see what kind of classical equations of motion we would get from the action (9). Without loss of generality, we can choose the field B to point in the z direction, $\boldsymbol{B} = B\hat{z}$. Then the action takes the form

$$S[\theta, \phi] = -\frac{\hbar}{2}\int_0^T dt[\dot{\phi}(1-\cos\theta) + \gamma B\cos\theta] \tag{10}$$

The classical equations of motion are derived by replacing $\theta \mapsto \theta + \delta\theta$ and $\phi \mapsto \phi + \delta\phi$ and setting the linear terms in $\delta\theta$ and $\delta\phi$ to zero. This leads to

$$\delta S = -\frac{\hbar}{2}\int_0^T dt[\delta\phi\frac{d}{dt}\cos\theta + (\dot{\phi} - \gamma B)\sin\theta\delta\theta] \tag{11}$$

Setting the terms proportional to $\delta\theta$ and $\delta\phi$ to zero gives the equations

$$\theta(t) = \text{const.} = \theta(0), \qquad \dot{\phi}(t) = \gamma B = \omega \tag{12}$$

This describes spin precession around the z axis where the z-component $n_z = \cos\theta$ remains unchanged as a function of time while the x and y components rotate with frequency ω, $n_x = \sin\theta\cos\phi = \sin\theta\cos\omega t$ and $n_y = \sin\theta\sin\phi = \sin\theta\sin\omega t$. Thus, the classical equations of motion reproduce the physics of spin precession we obtained from the operator formalism. Note that the first term in the action was crucial to obtain this result. Without it, we would have obtained the wrong equation of motion $\sin\theta = 0$.

We discussed earlier that the path integral is an alternative formulation of the quantum theory which does not have to be derived from the operator formalism. In particular, the quantization of spin should be already built-in in the formalism not something we put by hand. However, it is not obvious where such quantization would emerge given that we are describing the spin using a classical unit vector $\hat{n}$. To make this question more precise, let us try to generalize the path integral (9) to a general spin $\hbar s$ without making any assumption that s is quantized. Clearly the potential energy part of the action will become $-\frac{\hbar}{2}\boldsymbol{B}\cdot\hat{n} \mapsto -\hbar s\boldsymbol{B}\cdot\hat{n}$. Now since the physics of spin precession should not depend on the magnitude of the spin, to reproduce the same equation of motion (12), we need to also replace $\frac{\hbar}{2}$ in the first term in the action by $\hbar s$. This leads to the action

$$S[\hat{n}(t)] = 2s\hbar\int_0^T dt[i\langle\hat{n}|\partial_t\hat{n}\rangle - \frac{\gamma}{2}\boldsymbol{B}\cdot\hat{n}] \tag{13}$$

We will now show that, due to some special properties of the first term in the action, the path integral defined by the action above only leads to a well-defined theory if s is integer or half-integer.

Let us now study the properties of this term in detail:

$$S_B[\hat{n}(t)] = 2i\hbar s\int_0^T dt\langle\hat{n}|\partial_t\hat{n}\rangle = -\hbar s\int_0^T dt\dot{\phi}(1-\cos\theta) \tag{14}$$

We first note that this term is real since $\langle\partial_t\hat{n}|\hat{n}\rangle^* = \langle\hat{n}|\partial_t\hat{n}\rangle = -\langle\partial_t\hat{n}|\hat{n}\rangle + \partial_t\langle\hat{n}|\hat{n}\rangle = -\langle\partial_t\hat{n}|\hat{n}\rangle$. Second notice that this term only depends on the path $\hat{n}$ takes but not how fast it does it. This can be seen by rescaling $t \mapsto \lambda t$ (with $\hat{n}(\lambda T) = \hat{n}_f$) which does not change the value of the expression. These terms are called geometric terms (in contrast to dynamical terms). The geometric meaning of this term can be made more obvious by noting that the velocity of a point moving on a sphere described by the unit vector $\hat{n}$ is $\dot{\hat{n}} = \dot{\phi}\sin\theta\hat{e}_\phi + \dot{\theta}\hat{e}_\theta$. This leads to the expression

$$S_B[\hat{n}(t)] = -\hbar s\int_0^T dt\,\dot{\hat{n}}\cdot\boldsymbol{A}[\hat{n}] = -\hbar s\int_{\hat{n}_i}^{\hat{n}_f} d\hat{n}\cdot\boldsymbol{A}[\hat{n}], \qquad \boldsymbol{A}[\hat{n}] = \frac{1-\cos\theta}{\sin\theta}\hat{e}_\phi \tag{15}$$

Notice that the potential $\boldsymbol{A}$ is singular at the south pole $\theta = \pi$. The form (15) makes it clear that S_B only depends on the trajectory taken by $\hat{n}$ but not how fast or slow it is traversed. Let us now consider the special case of $\hat{n}_f = \hat{n}_i$. Our theory should be valid for any initial and final values including when they are equal. In this case, we can rewrite the line integral in (15) using Stokes theorem as an integral over area enclosed by the path

$$S_B[\hat{n}(t)] = -\hbar s\int d\boldsymbol{S}\cdot\tilde{\boldsymbol{B}}, \qquad \tilde{\boldsymbol{B}} = \nabla\times\boldsymbol{A} = \hat{e}_r \tag{16}$$

Notice however that there is an ambiguity in the expression above: a closed path on the circle divides it into two areas (See Fig. 1). Each can be said to be 'enclosed' by it [1]. In order for the theory to be consistent, these two alternatives should be equivalent. Since the area needs to be taken with opposite sign for the two regions, the different between the two choices is

$$S_{B,2} - S_{B,1} = \hbar s\int_{\text{region},1} d\boldsymbol{S}\cdot\tilde{\boldsymbol{B}} + \hbar s\int_{\text{region},2} d\boldsymbol{S}\cdot\tilde{\boldsymbol{B}} = S_{B,1} - S_{B,2} = \hbar s\int_{\text{sphere}} d\boldsymbol{S}\cdot\tilde{\boldsymbol{B}} = 4\pi\hbar s \tag{17}$$

Although the difference is non-zero, we note that the action only affects the physics through the exponential factor $e^{\frac{i}{\hbar}S}$ which means that changes in the action by an integer multiple of $2\pi\hbar$ do not change the physics.

[1] Recall the proof of Stokes theorem which divides the area into small regions and show the cancellation of the curl between them

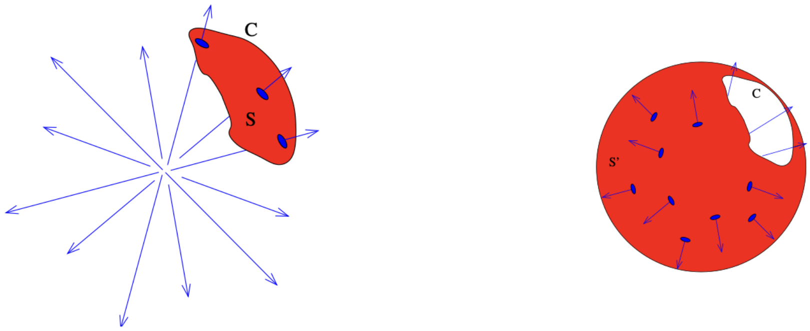

Figure 1: Illustration of the two possible choices of area on the unit sphere to compute the magnetic flux enclosed by a closed curve [Figure adapted from David Tong's lecture notes on Gauge theory]

This imposes the condition

$$4\pi\hbar s = 2\pi m\hbar, \qquad \Longrightarrow \qquad s = \frac{m}{2} \tag{18}$$

for m an arbitrary integer. Remarkably, we have derived the quantization of spin from the requirement that the path integral we derived is consistent!

In addition, you can convince yourself it is not gauge invariant; For example, under the transformation $|\hat{n}\rangle \mapsto e^{-i\phi}|\hat{n}\rangle$, this term changes to $\hbar s \int_0^T dt\dot{\phi}(1+\cos\theta)$. We see that the singularity is now at the north pole rather than the south pole. The difference between this new term and the original one for loops $n_i = n_f$ turns out to again given a factor of $4\pi\hbar s m$ that drops out from the path integral. For more general phases, it changes the action by a boundary term which yields an unimportant overall phase for the propagator.

There are a lot of deep and interesting physics hidden inside the term S_B. Let us first summarize what we learnt about its properties:

1. It depends on the path $\hat{n}(t)$ but not how fast it is traversed. We say such a term is geometric.
2. Its prefactor should be quantized to have a consistent theory
3. It is not gauge invariant in general. For paths starting and ending at the same point it changes by a multiple of $4\pi\hbar s$ which drops out of the amplitude for integer or half-integer s.
4. It describes the motion of a particle in a singular vector potential.

Each of these properties turn out to have far-reaching consequences beyond the specific example of the spin path integral that we will discuss during the next lecture.