LECTURE 1

§1. PATH INTEGRAL FOR SPIN

In what follows we assume a knowledge of the usual representations for spin, of spin algebra, and of the elementary quantum dynamics of spin.
A question of great interest that was posed (but not answered) by Feynman, when first developed path integrals, was "how to formulate a path integral theory for spin?". The problem here is simply that path theory is based on a sum over classical paths for a system, assuming a Lagrangian or Hamiltonian written in terms of classical variables. However spin has no classical analogue, and so it was not clear where to start from.

Recall that the general form for the path integral is, for the 1-particle Green fn. between initial state $|\psi_i\rangle$ and final state $|\psi_f\rangle$:

$$\left.\begin{aligned} G_{fi}(t_f,t_i) &\equiv \langle\psi_f|\hat{U}(t_f,t_i)|\psi_i\rangle \\ &= \int dq_1 \int dq_2 \, \langle\psi_f|q_2\rangle \; G(q_2,q_1;t_f,t_i) \, \langle q_1|\psi_i\rangle \end{aligned}\right\} \quad (1)$$

where in the "classical basis" of states $|q\rangle$, ie states corresponding to classical trajectories $q(t)$, we have the propagator

$$G(q_2 q_1; t_f, t_i) = \int_{x(t_i)=q_1}^{x(t_f)=q_2} \mathcal{D}x(\tau) \, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} d\tau \, L(x,\dot{x};\tau)} \qquad (2)$$

If we want to carry this formalism over to spin, we need to (i) find out what sort of states we can use that correspond to classical states; and (ii) find out the correct Lagrangian in terms of these states. In retrospect the answer seems obvious, but it was a long time in coming:

- Define the "classical states" as the coherent states $|\underline{\Omega}\rangle$ for spin that we have already defined.

- Assume a Lagrangian of the same form as that of a classical angular momentum.

Thus we write the propagator between initial and final spin states $|\psi_i\rangle$, $|\psi_f\rangle$ in the form

$$G_{fi}(t_f,t_i) = \int d\underline{\Omega}_1 \int d\underline{\Omega}_2 \, \langle\psi_f|\underline{\Omega}_2\rangle \; G(\Omega_2,\Omega_1;t_f,t_i) \, \langle\underline{\Omega}_1|\psi_i\rangle \qquad (3)$$

where the path integral for G_{21} is (PTO):

$$G(\underline{n}_2, \underline{n}_1; t_f, t_i) = \int_{\underline{\Omega}(t_1)=\underline{n}_1}^{\underline{\Omega}(t_2)=\underline{n}_2} \mathcal{D}\underline{\Omega}(\tau)\, e^{i/\hbar \int_{t_i}^{t_f} d\tau\, L(\underline{\Omega}, \dot{\underline{\Omega}}; \tau)} \qquad (4)$$

where $\underline{\Omega}(\tau)$ is a path on the Bloch sphere, defined by

$$\underline{\Omega}(\tau) = \langle \underline{\Omega}(t) | \hat{\underline{S}} | \underline{\Omega}(t) \rangle \qquad (5)$$

in terms of the coherent states directed along $\underline{\Omega}(t)$.

To get the correct form of the Lagrangian, we start from the equation of motion for a classical angular momentum $\underline{L}(t)$, given by

$$\frac{d\underline{L}}{dt} = -\underline{L}(t) \times \frac{\partial H}{\partial \underline{L}} \equiv -\underline{L}(t) \times \underline{T}(t) \qquad (6)$$

where $\underline{T}(t)$ is the instantaneous torque acting on the angular momentum. Consider now the Lagrangian:

$$L(\underline{n}, \dot{n}; t) = S\underline{A} \cdot \frac{d\underline{n}(t)}{dt} - \mathcal{H}(S\underline{n}; t) \qquad (7)$$

where $\mathcal{H}(S\underline{n})$ is the Hamiltonian, in which the operator $\hat{\mathcal{H}}(\hat{\underline{S}})$, a function of the operator $\hat{\underline{S}}$, is replaced by the same function of the classical vector $S\underline{n}$; and the vector $\underline{A}$ is the gauge potential due to a unit monopole at the centre of the unit Bloch sphere. This means that the field $\nabla \times \underline{A}$ is of unit magnitude along the radial direction on the Bloch sphere, ie, that

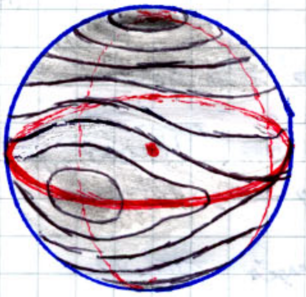
$$\underline{n} \cdot (\nabla \times \underline{A}) \equiv n_\alpha \epsilon^{\alpha\beta\gamma} \frac{\partial A_\beta}{\partial n_\gamma} = 1 \qquad (8)$$

We have already looked at the problem of a particle moving in the field of a monopole. The vector potential can be written in various ways – as we saw previously, 2 common forms are

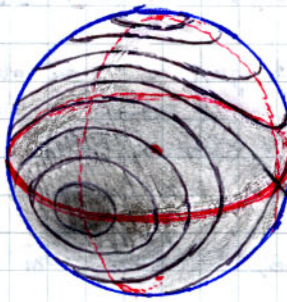
$$\underline{A}(\theta, \phi) = \left\{ \begin{array}{c} -\hbar \hat{\phi} \cot \theta/2 \\ -\hbar \hat{\phi} \dfrac{1 + \cos\theta}{\sin\theta} \end{array} \right\} \qquad (9)$$

in which the "Dirac string" comes in via the north pole of the Bloch sphere. In the present case we quantize the monopole strength in units of $\hbar$; this one has a strength $\hbar$. To conform with the Lagrangian (7) this then means we must give the particle moving on the Bloch sphere, at a coordinate $n(t)$, a "charge" of S.

The "potential" $\mathcal{H}(S\underline{n})$, also defined on the surface of the Bloch sphere, is a polynomial of order $2S+1$ in the variables S_x, S_y, and S_z; the terms allowed in this polynomial depend on the symmetries of the physical system – a topic which can be discussed exhaustively using group theory. Typically inversion symmetry is obeyed; it is sometimes useful to think about simple examples for $\mathcal{H}(\underline{S}_n)$, and so we will look at several of these, including:



(i) EASY PLANE, HARD AXIS



(ii) EASY AXIS, HARD AXIS

(i) A biaxial quadratic Hamiltonian with easy XY plane & hard X-axis; the Hamiltonian is

$$\left.\begin{aligned} \mathcal{H}_0 &= K_2^{\parallel} S_z^2 + K_2^{\perp}(S_x^2 - S_y^2) \\ &= K_2^{\parallel} S^2 \cos^2\theta + K_2^{\perp} S^2 \quad 2\phi \end{aligned}\right\} \quad (10)$$

where $K_2^{\parallel}, K_2^{\perp} > 0$ (11)

If we let $K_2^{\perp} \to 0$ in this Hamiltonian, then S_z is conserved, and the contours of equal potential just become "lines of latitude", with the highest potential at the north and south poles, and the equator forming a 1-d circular well.

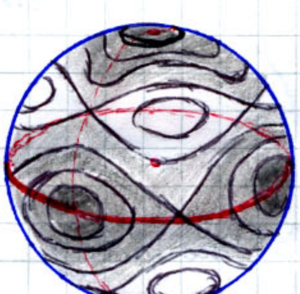
(ii) A biaxial quadratic Hamiltonian with hard Z-axis and hard X-axis; the Hamiltonian can then be written as

$$\left.\begin{aligned} \mathcal{H}_0 &= -K_2^{\parallel} S_z^2 + K_2^{\perp}(S_x^2 - S_y^2) \\ &\text{with} \quad K_2^{\parallel}, K_2^{\perp} > 0 \end{aligned}\right\} \quad (12)$$

and now the north and south poles are potential wells, and the highest potential is along the X-axis. If $K_2^{\perp} > 0$, the equator becomes a 1-d circular barrier.

(iii) Now choose a quartic Hamiltonian, which can in principle give us a wide variety of potential forms depending on the magnitude and sign of the coefficients. We pick the form

$$\left.\begin{aligned} \mathcal{H}_0 &= K_2^{\parallel} S_z^2 + K_2^{\perp}(S_+^2 + S_-^2) + K_4^{\parallel} S_z^4 + K_4^{\perp}(S_+^4 + S_-^4) \\ &\equiv S^2[K_2^{\parallel}\cos^2\theta + K_2^{\perp}\cos 2\phi] + S^4[K_4^{\parallel}\cos^4\theta + K_4^{\perp}\cos 4\phi] \end{aligned}\right\} \quad (13)$$



(iii) THE POTENTIAL IN EQTN (13), WITH $K_2^{\parallel}, K_4^{\perp} > 0$, $K_4^{\parallel} < 0$ AND $K_2^{\perp} = 0$.

Of the many possible forms, we show one at left with a set of potential wells strung out in the mid latitudes, along with 4 potential hills on the equator and one at each pole. The size of each potential hill and well is independent of ϕ; this is because we have chosen $K_2^{\perp} = 0$. If it were non-zero then only wells and hills differing by $180°$ in ϕ would be the same (ie., one would alternate between small and large wells & hills when circulating around the system at constant θ).

To any of these potentials we can also add an external field, which in principle will vary in time, ie in general we will have

$$\mathcal{H}(S\underline{n};t) = \mathcal{H}_0(S\underline{n}) - \gamma S\underline{n}\cdot\underline{H}_0(t) \tag{14}$$

We pause briefly here to note that, just as for any other problem in quantum mechanics, there is no classical analogue for sub-barrier tunneling or supra-barrier reflection – these will not appear in any classical equation of motion. However, just as in ordinary QM, they can be handled in path integral theory using instanton techniques.

In any case, in the classical regime, it follows from Lagrange's eqtns, viz.

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{n}}\right) - \frac{\partial L}{\partial \underline{n}} = 0 \tag{15}$$

that the eqtn of motion for $\underline{n}(t)$ is

$$\dot{n}(t) = -\underline{n}(t) \times \frac{\partial \mathcal{H}}{\partial \underline{n}} \tag{16}$$

with $\mathcal{H}(\underline{n},t)$ given by (14) above, and L given by (7). Notice a very important point – the "kinetic" or "topological" term in (7), which is linear in time derivatives, plays no role in this classical equation of motion.

Now let us construct the path integral for spins in the same way as one would for a particle, starting from the Green function written in terms of the unitary time evolution operator:

$$\left.\begin{aligned} G(\underline{n}_2,\underline{n}_1;t_2,t_1) &= \langle \underline{n}_2 | \hat{U}(t_2,t_1) | \underline{n}_1 \rangle \\ &\equiv \langle \underline{n}_2 | \hat{T}_\tau \exp \frac{-i}{\hbar}\int_{t_1}^{t_2} d\tau\, H(\tau) | \underline{n}_1 \rangle \end{aligned}\right\} \tag{17}$$

where $\hat{T}_\tau$ is the usual time-ordering operator, ie., we have

$$G(\underline{n}_2,\underline{n}_1;t_2 t_1) = \lim_{N\to\infty} \left(\frac{2S+1}{4\pi}\right)^N \prod_{j=1}^{N-1} \int d\underline{\Omega}_j \langle \underline{\Omega}_{j+1} | e^{-i/\hbar\, \mathcal{H}(t_j)\, dt} | \underline{\Omega}_j \rangle \tag{18}$$

Consider now the Green function defined over the

$$\left.\begin{aligned} \langle \Omega_{j+1} | U(t_j+\delta t, t_j) | \underline{\Omega}_j \rangle &= \langle \underline{\Omega}_{j+1} | e^{-i/\hbar\, \mathcal{H}(t_j)\, dt} | \underline{\Omega}_j \rangle \\ &= \langle \Omega_{j+1} | \underline{\Omega}_j \rangle \langle \underline{\Omega}_j | e^{-i/\hbar\, \mathcal{H}(t_j)\, dt} | \underline{\Omega}_j \rangle \end{aligned}\right\} \tag{19}$$

Thus we need the overlap integral $\langle \Omega_{j+1} | \underline{\Omega}_j \rangle$. Using the overlap integral

$$\langle \underline{n}_\alpha | \underline{n}_\beta \rangle = \left(\frac{1+\underline{n}_\alpha\cdot\underline{n}_\beta}{2}\right)^S e^{iS\Gamma_{\alpha\beta}} \tag{20}$$

where the angle $\Gamma_{\beta\alpha}$ is given by

$$\tan \tfrac{1}{2}\Gamma = \tan\left(\frac{\phi_\alpha - \phi_\beta}{2}\right) \frac{\cos\left(\frac{\theta_\alpha + \theta_\beta}{2}\right)}{\cos\left(\frac{\theta_\alpha - \theta_\beta}{2}\right)} \qquad (21)$$

we expand to 1st-order in dt, writing $|\underline{\Omega}(t_j + dt)\rangle = |\underline{\Omega}(t_j)\rangle (1 + \dot{\Omega}(t_j)\, dt)$ so that

$$\left.\begin{aligned} \langle \underline{\Omega}_{j+1} | \underline{\Omega}_j \rangle = \langle \underline{\Omega}(t_j + dt) | \Omega(t_j) \rangle &= e^{i(\dot{\phi}(t_j)\cos\theta(t_j))\, dt} \\ &\equiv e^{iS\underline{A}\cdot\dot{\underline{n}}(t_j)\, dt} \end{aligned}\right\} \qquad (22)$$

Thus we finally have

$$G(\underline{n}_2, \underline{n}_1; t_2 t_1) = \lim_{N\to\infty} (2S+1)^N \prod_{j=1}^{N-1} \int \frac{d\Omega_j}{4\pi}\, e^{i/\hbar\, S[\underline{\Omega}(t_j)]} \qquad (23)$$

with

$$\left.\begin{aligned} S &= \int d\tau\, \mathcal{L}(n, \dot{n}; \tau) \\ &= \int d\tau \left[S\underline{A}\cdot\dot{n}(\tau) - \mathcal{H}(S\underline{n}; \tau) \right] \end{aligned}\right\} \qquad (24)$$

Thus we recover (4) and (7). We could have also derived this result from a phase space path integral, in the form

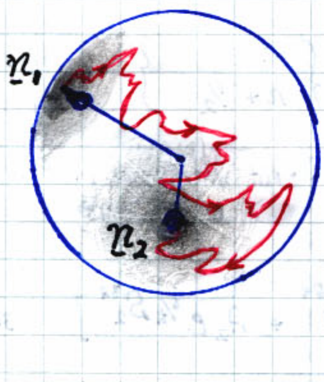
$$G(n_2, n_1; t_2 t_1) = \int_{p_1}^{p_2} \mathcal{D}p(\tau) \int_{q_2}^{q_1} \mathcal{D}q(\tau)\, e^{i/\hbar\, S[q,p]} \qquad (25)$$

if we identify the canonical variables p, q as

$$\left.\begin{aligned} p(\tau) &= S\cos\theta(\tau) \\ q(\tau) &= \phi(\tau) \end{aligned}\right\} \qquad (26)$$

so that

$$\left.\begin{aligned} S[q,p] &= \int d\tau\, [p\dot{q} - \mathcal{H}] \\ &= \int d\tau\, [S\dot{\phi}\cos\theta - \mathcal{H}] \end{aligned}\right\} \qquad (27)$$



We note that the paths are all defined on the Bloch sphere, and are subject to the same mathematical limitations as paths in ordinary space, in the usual Feynman path integral. However we should also note that, unlike the path integral in real space, the states $|\underline{\Omega}(t)\rangle$ on the Bloch sphere are not localised, ie., they are not δ-functions on the Bloch sphere.

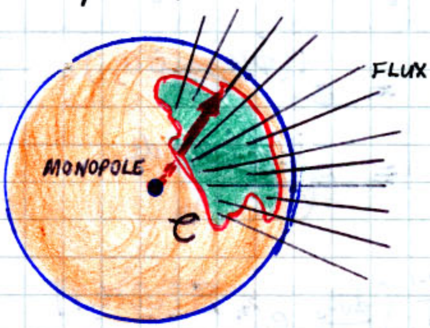
Let us now examine the most striking consequence of the result in (24). Integrating the 1st term, we have

$$\int_{t_1}^{t_2} dt\, S\underline{A}\cdot\dot{\underline{n}}(\tau) = \hbar S \tilde{\omega}_{21} \qquad (28)$$

where the total integral $\tilde{\omega}_{21}$ is
$$\hbar \tilde{\omega}_{21} = \int_{\underline{n}_1}^{\underline{n}_2} d\underline{n} \cdot \underline{A} \qquad (29)$$

Note again that since $\underline{A} \propto \hbar$, this integral, along the path of the system, disappears in the classical limit.

Because $\tilde{\omega}_{21}$ depends only on the path followed by the system, and not on the dynamics, it is clear that it is a geometric phase. In particular, if the path traced out is a closed circuit $\mathcal{C}$ on the Bloch sphere, then we immediately have



$$\hbar \tilde{\omega}_c = \oint_{\mathcal{C}} d\underline{n} \cdot \underline{A} \qquad (30)$$

and we see that $\tilde{\omega}_c$ is just the SOLID ANGLE swept out by the contour $\mathcal{C}$; and the geometric contribution to the action is just
$$\mathcal{S}_c = \hbar S \tilde{\omega}_c \qquad (31)$$

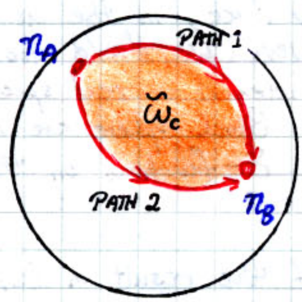
so that
$$G(\underline{n}_2, \underline{n}_1; t_2 t_1) = \int_{\underline{n}_1}^{\underline{n}_2} \mathcal{D}\underline{\Omega}(\tau)\, e^{iS\tilde{\omega}_{21}[\underline{\Omega}]}\, e^{-i/\hbar \int_{t_1}^{t_2} d\tau\, \mathcal{H}(\tau)} \qquad (32)$$

and for a closed circuit, the "return amplitude" is
$$G(\underline{n}, \underline{n}; t_2, t_1) = \oint_{\underline{n}} d\underline{\Omega}(\tau)\, e^{iS\tilde{\omega}_c[\Omega]}\, e^{-i/\hbar \int d\tau\, \mathcal{H}(\tau)} \qquad (33)$$

with a Berry phase
$$\phi_B = S \tilde{\omega}_c \qquad (34)$$

which is the product of the monopole flux $\hbar\tilde{\omega}_c$ through the area $\tilde{\omega}_c$ enclosed by the contour $\mathcal{C}$, and the charge S of the particle tracing out the contour, all divided by $\hbar$ (since $\phi_B = \mathcal{S}/\hbar$).

One immediate consequence of this result is that the spin can only take quantized values – the argument here is basically the same as that leading to monopole charge quantisation. The area $\tilde{\omega}_c$ is only defined modulo 4π, ie., the results should be unchanged under the transformation $\tilde{\omega}_c \to \tilde{\omega}_c + 4\pi m$, where m is any integer. We thus have
$$e^{4\pi i m S} = 1 \quad \Longrightarrow \quad S = \left\{ \begin{matrix} n \\ n + 1/2 \end{matrix} \right\} \qquad (35)$$



One can also imagine the analogue of 2-slit interference in spin space. Suppose the propagator between $|\underline{n}_A\rangle$ & $|\underline{n}_B\rangle$ is dominated by 2 paths, so that
$$\langle \underline{n}_B | \hat{U}(t_f, t_i) | \underline{n}_A \rangle \sim \left[A_1 e^{i/\hbar \mathcal{S}_1^{BA}} + A_2 e^{i/\hbar \mathcal{S}_2^{BA}} \right] \qquad (36)$$

and if $|A_1| = |A_2|$, the symmetric case, we get
$$\langle \underline{n}_B | \hat{U} | \underline{n}_A \rangle \longrightarrow A \cos \tilde{\omega}_c S \qquad (37)$$

where $\tilde{\omega}_c$ is now the area enclosed between the 2 paths. This is analogous to the problem of particles passing through 2 slits, when there is a flux $\Phi = S\tilde{\omega}_c$ enclosed between them. One can actually set up such a situation in spin space, by engineering the Hamiltonian so that the spin vector is forced along "potential valleys" by the potential $\mathcal{H}(\underline{S})$; moreover, these paths, and the enclosed area, can be controlled using external fields.

§2. SPIN DYNAMICS : THE SPIN - ½ CASE

As we saw previously, the most obvious thing to do once one has a formal expression for a path integral is to attempt a calculation of it, starting with an evaluation of the action along the classical path, and then looking for fluctuations around this. However in the case of spin there are 2 problems with this. The first is that the classical motion of an angular momentum under the action of forces / torques (or the motion of the charged particle in a combined monopole and potential field on a Bloch sphere) is extremely complex - the problem is highly non-linear. The second problem is that there is nothing in the classical solution to the eqtn. of motion (16) which can differentiate between different spins (ie., spins with different values of S), and yet we know that they behave quite differently in Q.M.

To get to grips with this we need to first study the Q.M. of the spin problem. This turns out to be much more complicated than one might imagine - and also highly non-linear.

2(a) WAVE - FUNCTION DYNAMICS

We consider the problem of a single spin - ½ in a time - dependent magnetic field, with Hamiltonian

$$\mathcal{H}(\underline{\sigma};t) \qquad \underline{B}(t)\cdot\hat{\underline{\sigma}} \tag{38}$$

where for the moment we place no restrictions on how $\underline{B}(t)$ varies in time. The eqtns of motion for the spin - ½ spinor wave - function $\chi_\sigma(t)$, from the Schrödinger eqtn.

$$\mathcal{H}\chi_\sigma(t) = i\hbar\partial_t\chi_\sigma(t) \tag{39}$$

are then

$$\left.\begin{aligned} i\hbar\dot{\chi}_+(t) &= B_z(t)\chi_+(t) + (B_x(t) + iB_y(t))\chi_-(t) \\ i\hbar\dot{\chi}_-(t) &= -B_z(t)\chi_-(t) + (B_x(t) - iB_y(t))\chi_+(t) \end{aligned}\right\} \tag{40}$$

Thus we have a coupled pair of 1st - order differential eqtns for $\chi_+(t)$ & $\chi_-(t)$, with time - varying coefficients. These are equivalent to a single 2nd - order differential equation, with the form (PTO):