SECTION D: SPIN AND ANGULAR MOMENTUM

The topic of spin is one of the most interesting in Quantum Mechanics; and both spin and angular momentum are full of hidden subtleties, many of which are only being explored now.

We note first that spin itself has no classical analogue; if we take the limit $\hbar \to 0$, then it disappears completely (this is of course not true for angular momentum). This means that the quasiclassical limit is not obvious, and indeed it was only in the 1980's that the formulation of a path integral for spin was given properly. The properties of the spin path integral are still somewhat mysterious.

In fact this is just the beginning of the subtleties associated with spin and angular momentum in Q.M. The path integral formulation of spin dynamics brings out the crucial role of topology in the problem - this appears both in the compact geometry, and in the way spin phase enters into the dynamics. However one can even see by examining the Schrödinger equation how different spin dynamics is from ordinary particle dynamics - in fact even quite apparently trivial problems in spin dynamics are unsolvable, and exhibit very peculiar behaviour, in marked contrast to, eg., the harmonic oscillator subject to various complicated forces. This is true even for a simple spin ½. For this reason the study of simple model problems is unusually interesting, using both perturbative & non-perturbative methods.

The subtleties of spin dynamics become of quite extraordinary subtlety, and unusually rich in physics, when we consider pairs of interacting spins. We will focus here on some aspects of the spin dynamics, with particular application to problems in atomic & molecular physics, and in quantum magnetism. We then move on to look at applications to quantum information processing, decoherence, and large-scale quantum phenomena: the spin dynamics of a pair of coupled spins leads us to some of the deepest questions in Quantum Mechanics.

D.1. SPIN PATH INTEGRALS

This topic has an interesting history. When Feynman first formulated path integral theory he found that he couldn't do it for spin. Eventually, in 1979, a formulation was given by Klauder, but it was unsatisfactory in certain respects - a really clear formulation did not appear until the 1980's, in the hands of Berry, Haldane, etc., which relied partly on the formulation of spin coherent states given by Radcliffe and Perelomov at the beginning of the 1970's.

The key problem is to understand the classical limit, so we will begin by briefly recalling some salient features of the classical dynamics of angular momenta, and how they are applied to give a semi-classical description of spin dynamics in classical magnetism. We then go on to look at the path integral for spin, in its modern formulation, bringing out the key topological features, and the connection to Berry's phase. Finally, we go back and relate what we have found to the usual formulation, in terms of Schrodinger's equation.

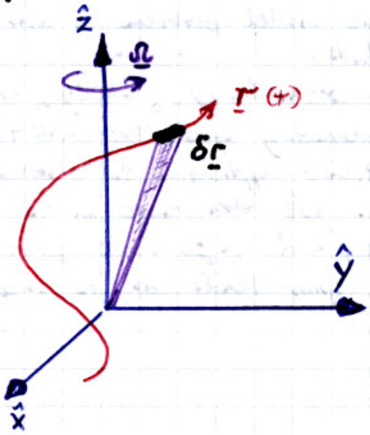
It is useful to recall the various representations used for spin in Quantum Mechanics. These are outlined in an Appendix. Apart from the usual operator algebra for spin & angular momentum, these representations include the coherent state rep., the bosonic reps. including Holstein-Primakoff and Schwinger bosons, and the Majorana representation.

D.1.1. CLASSICAL ANGULAR MOMENTUM

This topic is a standard part of undergraduate physics - however certain features acquire extra interest when they are viewed as the classical limit of the quantum theory of angular momentum. We begin by looking at some standard results for rotating classical bodies, and then recalling some simple features of the dynamics of magnetisation in the classical limit.

D.1.1(a) ROTATING CLASSICAL OBJECTS:

In any problem involving rotating objects, we first need to clarify the kinematics in a rotating frame.



Consider first a particle with trajectory $\underline{r}(t)$ in the "non-rotating" reference frame R. Then in a frame R' rotating with angular velocity $\underline{\Omega}$ (oriented along $\hat{z}$), so that

$$\underline{\Omega} = \hat{z}\Omega = \hat{z}\frac{d\phi}{dt} = \frac{d}{dt}\underline{\phi} \qquad (1)$$

where $\phi(t) = \Omega t$ is the total angle the frame R' has rotated w.r.t. R. Defining the velocity $\underline{v}(t) = \dot{\underline{r}}(t)$ in the inertial frame R, we then have in the frame R', that

$$\underline{v}'(t) = \underline{v}(t) - \underline{\Omega} \times \underline{r}(t) \qquad (2)$$

a result easily deduced by rewriting $\delta \underline{r} = \underline{v}\,\delta t$ in the rotating frame (for $\delta \underline{r}' = v'\,\delta t$).

From this we deduce the form of the Lagrangian and eqtns. of motion in the new frame. In the inertial frame we have, for a simple particle:

$$\mathcal{L} = \tfrac{1}{2}mv^2 - U(\underline{r}) \qquad (R) \qquad (3)$$

so that in the rotating frame we have

$$\mathcal{L}' = \tfrac{1}{2}mv'^2 + m\underline{v}' \cdot (\underline{\Omega} \times \underline{r}(t)) + \tfrac{1}{2}m(\underline{\Omega} \times \underline{r})^2 - U(\underline{r}) \qquad (4)$$

If we now use Lagrange's eqtns to find the eqtns of motion, we get

$$m\ddot{\underline{r}} = 2m(\dot{\underline{r}} \times \underline{\Omega}) + m\underline{\Omega} \times (\underline{r} \times \underline{\Omega}) - \frac{\partial U}{\partial \underline{r}} \qquad (5)$$

(CORIOLIS FORCE) (CENTRIFUGAL FORCE)

It is important to note the similarity, in L', between the effect of a a rotation and that of adding a gauge potential to the problem - we explore this further later on.

Rotation adds both a Coriolis force and a centrifugal force (the latter being the one that is often, in elementary texts, said not to exist!). The Coriolis force allows one to distinguish a rotating frame from an inertial one, by experiments done solely within that frame.

The Hamiltonian of the system is then

$$\mathcal{H}' = \dot{\underline{r}} \frac{\partial L'}{\partial \dot{r}} - L' \equiv E' \qquad (6)$$

$$= \tfrac{1}{2}mv^2 + \left(U(\underline{r}) - \tfrac{1}{2}m(\underline{\Omega} \times \underline{r})^2\right) \qquad (7)$$

Notice that this is NOT the same as the transformed kinetic energy minus the potential - we have

$$\left.\begin{aligned} \mathcal{H} &= T + V = \frac{\underline{p}^2}{2m} + V(r) \\ \text{where} \quad p &= m\underline{v} \end{aligned}\right\} \qquad (8)$$

whereas the transformed Hamiltonian reads

$$\mathcal{H}' = T' - m\underline{v}.(\underline{\Omega} \times \underline{r}) - m(\underline{\Omega} \times \underline{r})^2 + U(r) \qquad (9)$$

where T' is

$$T' = \tfrac{1}{2m}(\underline{p}')^2 \qquad (10)$$

and the transformed momentum is

$$\underline{p}' = \underline{p} + m(\underline{\Omega} \times \underline{r}) \qquad (11)$$

Note again the similarity with a gauge transformation. However this similarity is not exact - recall that in non-relativistic EM theory, one has a Lagrangian

$$L_{EM} = \tfrac{1}{2}m\dot{r}^2 + e\underline{A}(\underline{r}) \cdot \dot{\underline{r}} - e\phi(r) \qquad (12)$$

with a corresponding Hamiltonian

$$\left.\begin{aligned} \mathcal{H} &= \tfrac{1}{2m}(\underline{p} - eA(\underline{r}))^2 + e\phi(\underline{r}) \\ &= \tfrac{1}{2}m\dot{r}^2 + e\phi(\underline{r}) \end{aligned}\right\} \qquad (13)$$

with the generalised momentum

$$\underline{p} = \partial L / \partial \dot{\underline{r}} = m\dot{r} + eA(\underline{r}) \qquad (14)$$

Thus, if we pursue the analogy, we see that we can write the results in the transformed reference frame as follows; we define the "gauge potential"

$$\underline{A}_0(\underline{r}) = \underline{\Omega} \times \underline{r} \tag{15}$$

so that

$$\underline{p}' = \underline{p} + m\underline{A}_0(\underline{r}) = m\underline{v} + m\underline{A}_0(\underline{r}) \tag{16}$$

and then the Lagrangian transforms as

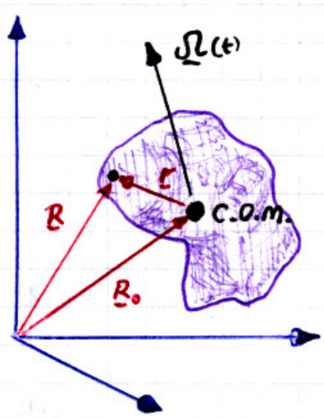
$$\mathcal{L} = \tfrac{1}{2}m\dot{r}^2 - U(r) \longrightarrow \mathcal{L}' = \tfrac{1}{2}m(\dot{\underline{r}}' + \underline{A}_0)^2 - U(\underline{r}) \tag{17}$$

and the Hamiltonian transforms as

$$\mathcal{H} = \frac{p^2}{2m} + U(r) \longrightarrow \mathcal{H}' = \frac{1}{2m}(\underline{p}' - m\underline{A}_0)^2 - U'_{eff}(\underline{r}) \tag{18}$$

where we now have an effective potential energy given by

$$\left.\begin{aligned} U'_{eff}(\underline{r}) &= U(r) - \tfrac{1}{2}mA_0^2(\underline{r}) \\ &= U(\underline{r}) - \tfrac{1}{2}m(\underline{\Omega}\times\underline{r})^2 \end{aligned}\right\} \tag{19}$$



Consider now a body in a reference frame considered to be static (& thus inertial), with density

$$\rho(\underline{R}) = \sum_{j=1}^{N} m_j\, \delta(\underline{R} - \underline{R}_j) \tag{20}$$

which we may take in the continuum limit (ie., $N \to \infty$, $m_j \to 0$) if we wish. The total mass is

$$M = \int d^3R\, \rho(\underline{R}) = \sum_j m_j \tag{21}$$

and the centre of mass is assumed to be at $\underline{R}_0$. From now on we define all positions $\underline{r} = \underline{R} - \underline{R}_0$ w.r.t. the centre of mass.

Let's assume the body is rotating about its c.o.m. with instantaneous angular velocity $\underline{\Omega}(t)$. It then follows that

$$\dot{\underline{R}}(t) = \dot{\underline{R}}_0(t) + (\underline{\Omega}(t) \times \underline{r}(t)) \tag{22}$$

and the kinetic energy of the system can be written as

$$\left.\begin{aligned} T = \tfrac{1}{2}\sum_j m_j \dot{R}_j^2 &= \tfrac{1}{2}\sum_j m_j \left[\dot{\underline{R}}_0 + (\underline{\Omega}(t)\times \underline{r}_j(t))\right]^2 \\ &= \tfrac{1}{2}M\dot{R}_0^2 + \tfrac{1}{2}\sum_j m_j \left[\Omega^2 r_j^2 - (\underline{\Omega}(t)\cdot\underline{r}_j(t))^2\right] \\ &= T_{com} + T_{Rot} \end{aligned}\right\} \tag{23}$$

where we use the vector identity $(\underline{a}\times\underline{b})^2 = a^2b^2 - (\underline{a}\cdot\underline{b})^2$, and note that by definition of the C.O.M., $\sum_j m_j r_j = 0$.

We now define the moment of inertia tensor for the solid body, in the usual way:

$$\left.\begin{aligned} I_{\alpha\beta} &= \sum_j m_j [r_j^2 \delta_{\alpha\beta} - r_j^\alpha r_j^\beta] \\ &\equiv \int d^3r \, \rho(r) \, [r^2 \delta_{\alpha\beta} - r^\alpha r^\beta] \end{aligned}\right\} \quad (24)$$

Then the angular momentum $\underline{L}^{rot}$ about the C.O.M. is defined as

$$L^\alpha_{rot} = I_{\alpha\beta} \Omega_\beta \quad (25)$$

and the rotational K.E. is $\quad T_{rot} = \frac{1}{2} \Omega_\alpha I_{\alpha\beta} \Omega_\beta \quad (26)$

Since $I_{\alpha\beta}$ is a symmetric tensor, we can diagonalize it by a rotation to principal axes.

We can summarize these results in the following formulae:

$$\left.\begin{aligned} T_{Rot} &= \tfrac{1}{2} \Omega_\alpha I_{\alpha\beta} \Omega_\beta = \tfrac{1}{2} \underline{L} \cdot \underline{\Omega} = \tfrac{1}{2} L_\alpha I^{-1}_{\alpha\beta} L_\beta \\ \mathcal{H}_{Rot} &= \underline{L} \cdot \underline{\Omega} - \mathcal{L}_{Rot} = \tfrac{1}{2} \Omega_\alpha I_{\alpha\beta} \Omega_\beta + U_{Rot} \\ &= \tfrac{1}{2} L_\alpha I^{-1}_{\alpha\beta} L_\beta + U_{Rot} \end{aligned}\right\} \quad (27)$$

where the Lagrangian $\quad \mathcal{L}_{Rot} = T_{Rot} - U_{Rot} \quad (28)$

and U_{Rot} is the potential acting on the rotational degrees of freedom

D.1.1.(b) CLASSICAL SPIN DYNAMICS

: We begin by considering the equations of motion for a spin or angular momentum in both the quantum and classical problems. To do this it is useful to refer to a simple Hamiltonian - we will assume we are dealing with a single spin $\underline{S}$, with Hamiltonian

$$\mathcal{H} = -\gamma \underline{S} \cdot \underline{H}_0 + V(\underline{S}) \quad (29)$$

where $V(\underline{S})$ is in general a polynomial in the components of $\underline{S}$ in the quantum problem, of maximal degree $2S$; in the classical problem it may have any form in $\underline{S}$ that is consistent with the symmetry of the problem.

In Q.M., we solve the dynamics of this system using the eqtn. of motion

$$i\hbar \dot{\hat{\underline{S}}} = [\hat{\underline{S}}, \hat{\mathcal{H}}] \quad \text{(Quantum)} \quad (30)$$

There is no immediately obvious relationship between this quantum equation, and the analogous classical equation for angular momentum dynamics, which is well known from classical mechanics to be

$$\dot{\underline{S}} = \hbar S \dot{\underline{n}} = -\frac{\partial V(\underline{n})}{\partial \underline{n}} \qquad (31)$$

where $\underline{n}$ is the unit vector in the direction of $\underline{S}(t)$. There are various ways of writing this equation of motion. If we start from Lagrange's eqtns for $\underline{n}(t)$, for either a spin $\underline{S} = \hbar S \underline{n}$, or an angular momentum $\underline{L}(t) = \hbar L\, \underline{n}(t)$, we have

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{n}}\right) - \frac{\partial L}{\partial \underline{n}} \qquad (32)$$

and since from (25)-(28) above we have, for the classical system

$$\left.\begin{aligned} L(n,\dot{n}) &= \tfrac{1}{2}\, \dot{n}_\alpha I_{\alpha\beta}\, \dot{n}_\beta - V(\underline{n}S) \\ &\equiv \tfrac{1}{2}\, \underline{S}_\alpha \cdot \dot{\underline{n}}_\beta - V(\underline{n}S) \end{aligned}\right\} \qquad (33)$$

where we define the classical spin (in analogy with a classical angular momentum) by

$$\underline{S}_\alpha = I_{\alpha\beta}\, \dot{\underline{n}}_\beta \qquad (34)$$

in terms of a moment of inertia. Substituting (33) into (32), we get (31). Alternatively, we can write the equation of motion as

$$\left.\begin{aligned} \dot{\underline{S}} &= -\underline{S}(t) \times \frac{\partial V(\underline{S})}{\partial \underline{S}} \\ \hbar S \dot{\underline{n}} &= -\underline{n}(t) \times \frac{\partial V(\underline{n})}{\partial \underline{n}} \end{aligned}\right\} \qquad (35)$$

because the magnitude S is conserved. Another way of writing the eqtn of motion arises when we are able to write the potential $V(\underline{S})$ in the form

$$V(\underline{S}) = -\gamma \underline{S} \cdot \underline{H}_{eff} \qquad (36)$$

where we think of $\underline{H}^{eff}$ as an "effective magnetic field"; it then follows that

$$\dot{\underline{S}} = \gamma\left(\underline{H}_{eff} \times \underline{S}(t)\right) \qquad (37)$$

This equation is of considerable application in the theory of classical magnetization dynamics, where one defines a classical vector $\underline{M}(\underline{r},t)$ intended to represent a "coarse-grained" average magnetic moment. In this case the Hamiltonian typically takes a form like

$$\mathcal{H}_{eff}[\underline{M}] = \int d^3r \Big\{ \tfrac{1}{2}\Big[J_{ij}^{\alpha\beta} \nabla_i M^\alpha(\underline{r}) \nabla_j M^\beta(\underline{r}) + K_{\alpha\beta} M^\alpha(\underline{r}) M^\beta(\underline{r}) \Big] - (\underline{H}_0 + \underline{H}_{dp}(\underline{r})) \cdot \underline{M}(\underline{r}) + O(M^4) \Big\} \quad (38)$$

where $J_{\alpha\beta}$ is an exchange coupling, $K_{\alpha\beta}$ is an anisotropy energy, H_0 an applied field, and $\underline{H}_{dp}(\underline{r})$ is a dipolar or "demagnetization" field, given by

$$\underline{H}_{dp}(\underline{r}) = -\nabla_r \int d^3r' \, \underline{M}(\underline{r}') \cdot \nabla_{r'} \frac{1}{|\underline{r}-\underline{r}'|} \quad (39)$$

ie., it is the total dipolar field generated at $\underline{r}$ by all the spins in the rest of the system. Clearly we can rewrite (38) as

$$\left.\begin{aligned} \mathcal{H}_{eff}[M] &= \int d^3r \, \underline{M}(\underline{r}) \cdot \underline{H}_{eff}(\underline{r}) \\ H^\alpha_{eff}(\underline{r}) &= H_0^\alpha + H_{dp}^\alpha(\underline{r}) + K_{\alpha\beta} M_\beta(\underline{r}) + J_{ij}^{\alpha\beta} \frac{\partial^2 M^\beta}{\partial r_i \, \partial r_j} \end{aligned}\right\} \quad (40)$$

where the last exchange term in $\underline{H}_{eff}(\underline{r})$ is obtained by integration by parts.

The equation of motion of a freely precessing magnetic moment is known from experiment (and is derivable from QED); one has

$$\dot{M} = g\mu_B (\underline{H}_0 \times \underline{M}) \quad (41)$$

where $\mu_B = \hbar e/2m$. From this it follows that: $\quad g\mu_B = \gamma \quad (42)$

in (37). In the same way, we can write a general eqtn. of motion for $\underline{M}(t)$, in the form

$$\underline{\dot{M}}(t) = -\gamma \left(\underline{M}(t) \times \frac{\partial \mathcal{H}^{eff}[M]}{\partial \underline{M}} \right) \quad (43)$$

So far, so good. However this derivation does not actually give us the Lagrangian for a quantum spin - the moment of inertia in (33) and (34) is meaningless for a quantum spin.

To address this problem, a form for the Lagrangian was used in the 1960's and following, of form

$$\mathcal{L}[M,\dot{M}] = \int d^3r \, P(r,t) \dot{Q}(r,t) - \mathcal{H}_{eff}[M] \quad (44)$$

with

$$\left.\begin{aligned} P(\underline{r},t) &= \frac{|M(r,t)|}{\gamma} \cos\theta(r,t) \\ Q(\underline{r},t) &= \varphi(r,t) \end{aligned}\right\} \quad (45)$$

in which θ, φ parametrize the orientation of $\underline{M}(r,t)$:

$$\left.\begin{aligned} \underline{M}(r,t) &= |M(r,t)|\, \underline{n}(r,t) \\ \underline{n}(r,t) &= (\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta) \end{aligned}\right\} \quad (46)$$

We treat $P(\underline{r},t)$ and $\Phi(\underline{r},t)$ as canonical variables, so that Hamilton's eqtns read :

$$\left.\begin{aligned} \dot{P} + \partial\mathcal{H}^{eff}/\partial\Phi &= 0 \\ \dot{Q} - \partial\mathcal{H}^{eff}/\partial P &= 0 \end{aligned}\right\} \quad (47)$$

which immediately gives us the Landau-Lifshitz eqtn in (43).

Thus the Lagrangian in (44) gives the correct equation of motion for $\underline{M}$, under the assumption that $|M(\underline{r},t)|$ is conserved (not necessarily a good assumption in a magnetic system. However (44) is not entirely satisfactory - in particular, it singles out a particular axis (the $\hat{z}$-axis) for special consideration, a procedure unjustified by the symmetry of the problem.

D.1.2. SPIN PATH INTEGRAL

A satisfactory derivation of a path integral for spin had to wait for the formulation of a "coherent state" formalism for spin, given in an Appendix to these notes. Once this was done it was possible to write the propagator between two spin states $|\psi_{in}\rangle$ and $|\psi_f\rangle$ as

$$\left.\begin{aligned} \langle\psi_f|\hat{G}(t_2t_1)|\psi_{in}\rangle &= G_{fi}(t_2,t_1) \\ &= \int d^2\underline{n}_1 \int d^2\underline{n}_2\ \langle\psi_f|\underline{n}_2\rangle\langle\underline{n}_2|\hat{G}(t_2t_1)|\underline{n}_1\rangle\langle\underline{n}_1|\psi_{in}\rangle \end{aligned}\right\} \quad (48)$$

where the propagator $G(\underline{n}_2,\underline{n}_1;t_2,t_1)$ between coherent states $|\underline{n}_1\rangle$ and $|\underline{n}_2\rangle$ can be written as a path integral :

$$\left.\begin{aligned} \langle\underline{n}_2|\hat{G}(t_2t_1)|\underline{n}_1\rangle &= G(\underline{n}_2,\underline{n}_1;t_2,t_1) \\ &= \int_{\underline{\Omega}(t_1)=\underline{n}_1}^{\underline{\Omega}(t_2)=\underline{n}_2} \mathcal{D}\underline{\Omega}(\tau)\ e^{i/\hbar \int_{t_1}^{t_2} d\tau\, L(\underline{\Omega},\dot{\underline{\Omega}};\tau)} \end{aligned}\right\} \quad (49)$$

Unlike the standard case, where we already know the Lagrangian for the system, and we calculate the path integral directly, in this problem the Lagrangian is not known. However what we can do is <u>derive</u> the Lagrangian, in a rather back-handed way, by deriving the path integral in the form (49) by starting from the Hamiltonian (which we do know).

To do this we follow the by now standard routine of splitting the path integral, now defined in terms of the unitary time evolution operator, into an infinite set of infinitesimal segments, each of which is sandwiched between coherent spin states.

Thus we start from

$$\left.\begin{aligned} G(\underline{n}_2\underline{n}_1;t_2t_1) &= \langle \underline{n}_2 | \hat{U}(t_2,t_1) | \underline{n}_1 \rangle \\ &\equiv \langle \underline{n}_2 | \hat{T}_\tau \exp\left\{-\tfrac{i}{\hbar}\int_{t_1}^{t_2} d\tau\, \mathcal{H}(\tau)\right\} | \underline{n}_1 \rangle \end{aligned}\right\} \quad (50)$$

where $\hat{T}_\tau$ is the time-ordering operator; and so we have, upon chopping up the time integration in (50), that

$$G(\underline{n}_2,\underline{n}_1;t_2t_1) = \lim_{N\to\infty} \left(\frac{2S+1}{4\pi}\right)^N \prod_{j=1}^{N-1} \int d\underline{\Omega}_j \langle \underline{\Omega}_{j+1} | e^{-\frac{i}{\hbar}H(t_j)dt} | \underline{\Omega}_j \rangle \quad (51)$$

where the $|\underline{\Omega}_j\rangle$ are coherent spin states. The propagator between the states $|\underline{\Omega}_j\rangle$ and $|\underline{\Omega}_{j+1}\rangle$, over an infinitesimal time interval, is

$$\left.\begin{aligned} \langle \underline{\Omega}_{j+1} | \mathcal{U}(t_j+dt,t_j) | \underline{\Omega}_j \rangle &= \langle \underline{\Omega}_{j+1} | e^{-\frac{i}{\hbar}\mathcal{H}(t_j)dt} | \underline{\Omega}_j \rangle \\ &= \langle \underline{\Omega}_{j+1} | \underline{\Omega}_j \rangle \langle \underline{\Omega}_j | e^{-\frac{i}{\hbar}\mathcal{H}(t_j)dt} | \underline{\Omega}_j \rangle \end{aligned}\right\} \quad (52)$$

Thus we need the overlap integral $\langle \underline{\Omega}_{j+1} | \underline{\Omega}_j \rangle$. From the appendix, we have, for 2 coherent states $|\underline{\Omega}_\alpha\rangle$ and $|\underline{\Omega}_\beta\rangle$, that

$$\left.\begin{aligned} \langle \underline{\Omega}_\alpha | \underline{\Omega}_\beta \rangle &= \left(\frac{1+\underline{\Omega}_\alpha\cdot\underline{\Omega}_\beta}{2}\right)^S e^{iS(\Gamma_{\alpha\beta}+\chi_\alpha-\chi_\beta)} \\ \tan\tfrac{1}{2}\Gamma_{\alpha\beta} &= \tan\left(\frac{\varphi_\alpha-\varphi_\beta}{2}\right) \frac{\cos\left(\frac{\varphi_\alpha+\varphi_\beta}{2}\right)}{\cos\left(\frac{\varphi_\alpha-\varphi_\beta}{2}\right)} \end{aligned}\right\} \quad (53)$$

Using now the infinitesimal character of $\underline{\Omega}_{j+1}-\underline{\Omega}_j$, we expand everything to 1st order in dt, so that

$$|\underline{\Omega}_{j+1}\rangle = (1+\dot{\underline{\Omega}}_j\, dt)\,|\underline{\Omega}_j\rangle \quad (54)$$

so that

$$\langle \underline{\Omega}_{j+1} | \underline{\Omega}_j \rangle = 1 + iS\left(\dot{\varphi}(t_j)\cos\theta(t_j) + \dot{\chi}(t_j)\right) dt \quad (55)$$

We note 2 things about this result. First, the dependence on $\dot{\varphi}\cos\theta$ arises ultimately from the special choice of coordinates, referring back to the $\hat{z}$-axis and rotations away from it, in our definition of spin coherent states. One should recognize that the actual result for $\langle \underline{\Omega}_\alpha | \underline{\Omega}_\beta \rangle$, in a manifestly rotation invariant formalism, cannot depend on the angle $\cos\Theta$ that each is rotated away from the $\hat{z}$-axis, but only on the difference $d\Omega = \Omega_\alpha - \Omega_\beta$. To show this explicitly it is necessary to set up the coherent state formalism in a rotationally invariant way, using the language of differential forms, which we do not do here.

Nevertheless it is obvious that what we are actually dealing with in (55) is an increment in area — which only appears explicitly if we make a series of infinitesimal changes in Ω which ultimately bring it back to itself. We thus think of

$$(d\varphi \cos\theta + d\chi) \equiv d\omega \tag{56}$$

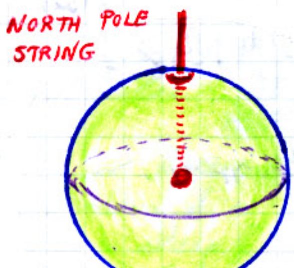
and we see that we can write

$$d\omega \equiv \underline{A} \cdot d\underline{n} \tag{57}$$

where A is the vector potential of a unit monopole, introduced before in section II, and defined here by

$$\underline{n} \cdot (\nabla \times \underline{A}) = n_\alpha \epsilon^{\alpha\beta\gamma} \frac{\partial A^\beta}{\partial n^\gamma} = 1 \tag{58}$$

In the convention chosen for coherent states where angles are referred to the $\hat{z}$-axis, we choose the Dirac string to go through the north pole. Then we can write various forms for $\underline{A}$ with this choice; we recall two of them here:



$$\underline{A}(\theta,\phi) = \left\{ \begin{array}{c} -\hat{\phi} \cot \theta/2 \\ \\ -\hat{\phi}\, \dfrac{1+\cos\theta}{\sin\theta} \end{array} \right\} \tag{59}$$

where one can show that different gauge choices for $\underline{A}(\theta,\varphi)$, for this "north pole" configuration, actually correspond to different choices of χ.

If we now assume the validity of (57), we can write the overlap integral in (55) as

$$\langle \underline{\Omega}_{j+1} | \underline{\Omega}_j \rangle = 1 + iS\underline{A} \cdot \dot{\underline{n}}(t_j)\, dt \tag{60}$$

This brings us to our 2nd remark about (55); it is, by construction, the first term in the expansion of an exponential. Thus we can now construct the entire path entire path as follows:

$$\left. \begin{array}{l} G(\underline{n}_2, \underline{n}_1; t_2 t_1) = \lim\limits_{N\to\infty} (2S+1)^N \prod\limits_{j=1}^{N-1} \displaystyle\int \frac{d\Omega_j}{4\pi}\, e^{i/\hbar\, S[\Omega(t_j)]} \\ \\ S[\underline{\Omega}] = \displaystyle\int d\tau\, L(\Omega, \dot{\Omega}; \tau) = \int d\tau \left[\hbar S \underline{A} \cdot \dot{\underline{\Omega}}(\tau) - H(S\underline{\Omega}; \tau)\right] \end{array} \right\} \tag{61}$$

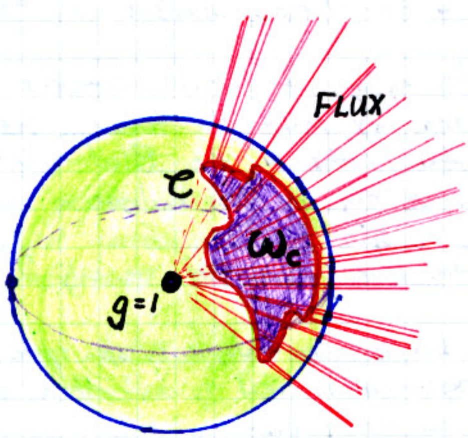
We note that this form for the Lagrangian reduces to that given in (44) and (45), provided we make the appropriate gauge choice. We could also have derived (44) and (45) by using a phase space path integral formulation, starting from

$$\left.\begin{aligned} G(\underline{n}_2,\underline{n}_1;t_2,t_1) &= \int_{P_1}^{P_2} \mathcal{D}P(\tau) \int_{Q_1}^{Q_2} \mathcal{D}Q(\tau)\, e^{i/\hbar S[P,Q]} \\ S(P,Q) &= \int d\tau \left[P\dot{Q} - \mathcal{H} \right] \end{aligned}\right\} \qquad (62)$$

and making the gauge choice $\left.\begin{aligned} P &= S\cos\theta \\ Q &= \varphi \end{aligned}\right\}$ (63)

Clearly one could redo the entire analysis in a more general gauge, in this phase space formulation – we do not go through this here.

It is clear now from the result in (61) that the "kinetic term" in the Lagrangian plays a very unusual role. Suppose we separate it out from the Hamiltonian term in the path integral, and write, for a path $\underline{n}(\tau)$, the Green function as



$$\left.\begin{aligned} G(\underline{n}_2,\underline{n}_1;t_2,t_1) &= \\ &\int_{n_1}^{n_2} \mathcal{D}\Omega(\tau)\, e^{iS\omega_{21}[\underline{n}]}\, e^{-i/\hbar \int d\tau \mathcal{H}(\tau)} \end{aligned}\right\} \quad (64)$$

where the scalar quantity ω_{21} is the integral along the curve $\underline{n}(\tau)$ of the kinetic term:

$$\omega_{21}[\underline{n}] = \int_{n_1}^{n_2} \underline{A}\cdot d\underline{\Omega} \Big|_{\Omega(\tau)=\underline{n}(\tau)} \qquad (65)$$

Now as it stands this quantity is gauge-dependent. In fact it looks exactly like the gauge-dependent term in the EM Lagrangian (12) for a charged particle, and we see that the Lagrangian in (61) is exactly that for a particle of charge $\hbar S$, interacting with the magnetic field from a UNIT monopole at the centre of a unit Bloch sphere, with the constraint that the charged particle must move on the surface of the sphere. We also note that the particle is massless – there is no kinetic term $\propto \dot{\underline{n}}^2$, like that in (12).

Consider now what happens if the particle completes a circuit on the Bloch sphere, so that we are looking at a return amplitude $G(\underline{n},\underline{n};t)$, for the particle to start and finish at $\underline{n}$. We then have

$$G(\underline{n},\underline{n};t) = \oint_{\mathcal{C}} d\Omega(\tau)\, e^{iS\omega_c}\, e^{-i/\hbar \int d\tau\, \mathcal{H}(\underline{\Omega},\tau)} \qquad (66)$$

with a Berry phase $\qquad \phi_B = S\omega_c \qquad (67)$

where ω_C is the area enclosed by the circuit $\mathcal{C}$ on the Bloch sphere. This is indeed a Berry phase - but we notice here that it is not derived in the adiabatic limit - there is no requirement that the circuit $\mathcal{C}$ be traversed slowly.

One very elegant consequence of this result is that it imposes an automatic quantization requirement on the spin. We use a similar argument to that for the derivation of the Dirac monopole condition (ie., that $eg = m\hbar$, where g is the monopole charge). The area ω_C is only defined modulo 4π, so that the results derived above should be unchanged under the transformation

$$\omega_C \rightarrow \omega_C + 4\pi m \tag{68}$$

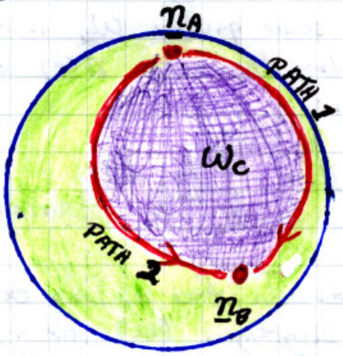
where m is an integer. We thus have

$$e^{4\pi i m S} = 1 \quad \Longrightarrow \quad \left\{ S = \begin{matrix} n \\ n+\frac{1}{2} \end{matrix} \right\} \tag{69}$$

where n is an integer. This does not tell us the statistics associated with the spins (for which we need QED).

In the same way, we can look at the analogue of 2-slit interference in spin space. Imagine a situation where a spin can only make the transition between 2 states $|\underline{n}_a\rangle$ and $|\underline{n}_b\rangle$ along certain paths on the Bloch sphere. If we can set up such a situation, then we can do the analogue of an Aharonov-Bohm experiment, but this time in spin space.

This is shown in the figure, in the case where there are only 2 allowed paths.



This situation is the analogue in spin space of a 2-slit experiment in real space, with an enclosed flux between the paths.

Suppose the propagator along the paths is given by

$$G_{BA}(t) = \left[A_1(t) e^{i/\hbar S_1^{BA}(t)} + A_2(t) e^{i/\hbar S_2^{BA}(t)} \right] \tag{70}$$

Now if the problem is not symmetric, $A_1 \neq A_2$, and $S_1^{BA} \neq S_2^{BA}$, in general. But one can arrange things so that the paths are symmetrically disposed about a plane of symmetry. Then we have

$$\left. \begin{matrix} |A_1| = |A_2| \\ S_1^{BA} = S_2^{BA} \end{matrix} \right\} \Longrightarrow \quad G_{BA}(t) \sim A(t) \cos \omega_C S \tag{71}$$

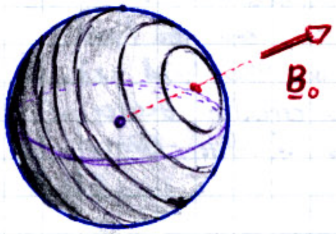
where $A(t)$ is some overall complex amplitude. In this case we see that the total amplitude shows interference oscillations between the paths, which suppress the amplitude to zero under the right conditions. Later on we will look in detail at experiments which look at this kind of spin interference phenomenon, where the paths are "tunneling paths" in spin space, enforced by the form of the Hamiltonian $\mathcal{H}(\underline{S})$.

Mention of the role of the Hamiltonian $\mathcal{H}(\underline{S})$ reminds us of the second crucial term in (61) and (64). Just as for the problem of a QM particle, path integral methods turn out to be terribly useful in understanding the way in which the form of $\mathcal{H}(\underline{S})$ influences $G_{21}(t)$. We will explore this in more detail below, but let's first do a quick survey of the kinds of Hamiltonian one might expect, and how they might influence the dynamics.

For simple spin Hamiltonians, the easiest way to classify them is by their symmetry. We note that a spin-½ system will have a trivial Hamiltonian: one has

$$\mathcal{H}(\tau) = -\frac{\gamma}{2}\underline{B}_0 \cdot \hat{\underline{\tau}} \qquad (\text{spin}-1/2) \qquad (72)$$

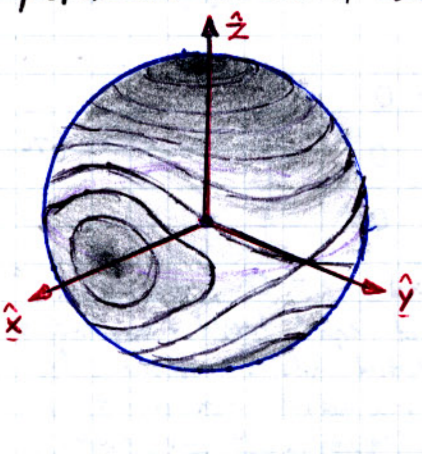
where $\underline{b}_0$ is a constant field. We assume $\gamma > 0$, so that the lowest energy state is oriented along $\underline{b}_0$. Then the diagram shows equipotential lines for the Hamiltonian, viewed now as a potential defined on the Bloch sphere - lower potential regions are shown more lightly shaded.



One can think of simple precessional motion - the natural motion of a spin in a static field, whether it be spin-½ or higher spin - as the motion of $\underline{n}$ along equipotentials (not perpendicular, as would happen if there was a genuine kinetic term $\sim \dot{\underline{n}}^2$). This motion along equipotentials is the result of combining the "potential" $\mathcal{H}(\underline{S})$ with the gauge term $\hbar\dot{\underline{S}}\cdot\underline{A}$; it is of course in accordance with the conservation of energy.

For higher spins one has more complex potentials. Here we consider 3 simple examples:

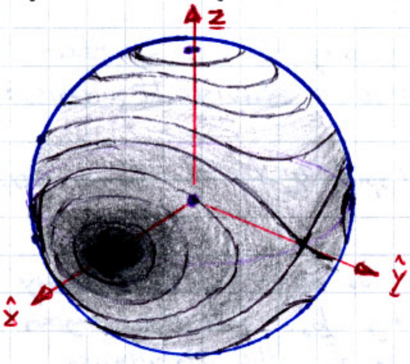
(1) <u>BIAXIAL, EASY PLANE</u> : We consider a system with 2 perpendicular axes of symmetry, in which an easy plane is perpendicular to one of these axes - we take this to be the $X.Y$-plane, so that the $\hat{z}$-axis is a hard axis. Then, in the easy plane, we also have an axis of symmetry, which we will choose to be the $\hat{x}$-axis, which we can with no loss of generality take to be another hard axis. We will assume the simplest possible such Hamiltonian, of quadratic form in the components of $\underline{S}$; then we have



$$\left.\begin{aligned} \mathcal{H}_0(\underline{S}) &= K_z S_z^2 + K_\perp (S_x^2 - S_y^2) \\ &\equiv S^2\left(K_z \cos^2\theta + K_\perp \sin^2\theta \cos 2\phi\right) \\ &\quad (\text{with } K_z, K_\perp > 0) \end{aligned}\right\} \quad (73)$$

Notice that if we let $K_\perp \to 0$, we get an easy plane system, with equipotentials along "lines of latitude" (with the poles at high energy). In this case the equator forms a circular potential well, ie., a 1-d periodic potential.

(ii) <u>BIAXIAL, EASY AXIS</u> : We can continuously deform the potential of (73) into an easy axis one, by changing the sign of the longitudinal term in (73). We now assume a potential of form

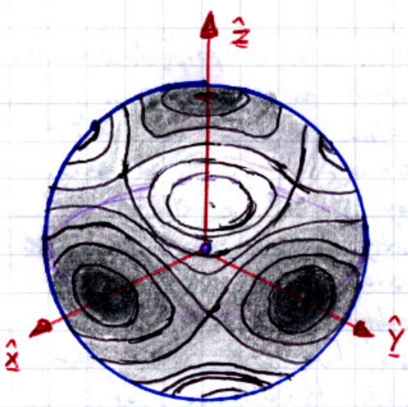


$$\left.\begin{aligned} \mathcal{H}_0(\underline{S}) &= -K_z S_z^2 + K_\perp (S_x^2 - S_y^2) \\ &\equiv S^2 (K_z \sin^2\theta + K_\perp \sin^2\theta \cos 2\phi) \\ &(K_z, K_\perp > 0) \end{aligned}\right\} \quad (74)$$

where we ignore irrelevant constant terms. Now the system has 2 potential wells at the north and south poles, and we have again made the x-axis the hard axis. If now let $K_\perp \to 0$, the equator becomes a symmetric circular barrier - otherwise, there are "saddle point" lowest regions of this barrier, along $\hat{\underline{y}}$ and $-\hat{\underline{y}}$.

(iii) <u>QUARTIC BIAXIAL SYSTEM</u> : Now we choose a Hamiltonian $\mathcal{H}_0(\underline{S}) \sim O(S^4)$, so that get a much wider variety of possible behaviours. Let's choose a system which again has biaxial symmetry, as above, and consider the form

$$\left.\begin{aligned} \mathcal{H}_0(\underline{S}) &= K_2^z S_z^2 + K_2^\perp (S_+^2 - S_-^2) + K_4^z S_z^4 + K_4^\perp (S_+^4 + S_-^4) \\ &\equiv S^2 \left[K_2^z \cos^2\theta + K_2^\perp \sin^2\theta \cos 2\phi \right] + S^4 \left[K_4^z \cos^4\theta + K_4^\perp \sin^4\theta \cos 4\phi \right] \end{aligned}\right\} (75)$$



There are so many different variants of this potential, that we plot a single one, and discuss in words how it is modified by changing the parameters. At left we show

$$\left.\begin{aligned} K_2^z, K_4^\perp &> 0 \\ K_4^z &< 0 \\ K_2^\perp &= 0 \end{aligned}\right\} \quad (76)$$

Because we have fixed $K_2^\perp = 0$, the 4 "hills" on the equator are of equal height - a non-zero value for $K_2^\perp$ would create pairs of equal potential hills on opposite sides of the equator, with unequal heights - so that one would alternate between large & small hills as one travelled around the equator. As one moves away from the equator, this 4-fold symmetric pattern of hills and wells persists. In the scheme shown, one has eight potential wells of equal depth, separated by 4 potential hills on the equator, and two at the poles. Obviously, by varying the parameter values, one can make the depths of the wells, and heights of the potentials, unequal (while still preserving the inversion symmetry), and also reverse the roles of hills and wells. Thus a huge variety of behaviours is possible in this quartic potential.

Now let us briefly return to the question of the relationship with the classical problem. Suppose we wish to recover some sort of classical behaviour for the spin dynamics from the path integral formulation just given - how do we do this, and what do we get?

In discussing particle dynamics, we saw that the classical limit was obtained by letting the action become very large - this could be accomplished either by having a large mass, or a very long trajectory with large energy.

To do something analogous with spin, the obvious thing to take is a large S limit, ie., consider

$$\lim_{S \gg 1} \mathcal{S}[\underline{n}] = \lim_{S \gg 1} \int_{t_1}^{t_2} d\tau \left[\hbar S \underline{A} \cdot \dot{\underline{n}}(\tau) - \mathcal{H}(S\underline{n};\tau) \right] \qquad (77)$$

and, in this limit, look for paths that extremize the action, ie., for which $\underline{n} \to \underline{n}_c$ such that:

$$\delta \mathcal{S}[n, \dot{n}] \Big|_{n = n_c} = 0 \qquad (78)$$

(cf section A.1.1 (a)); and we assume

$$\left. \begin{aligned} \underline{n}(t = t_1) &= \underline{n}_1 \\ \underline{n}(t = t_2) &= \underline{n}_2 \end{aligned} \right\} \qquad (79)$$

Expanding out (78) we find that

$$\delta \mathcal{S} = \hbar S \int_{t_1}^{t_2} dt \left[\left(\frac{\partial A^\alpha}{\partial n^\beta} \delta n^\beta \right) \dot{n}^\alpha + A^\alpha \frac{d}{dt} \delta n^\alpha \right] \Bigg|_{\underline{n} = \underline{n}_c} - \int_{t_1}^{t_2} d\tau \frac{\partial \mathcal{H}}{\partial n^\alpha} \delta n^\alpha \Bigg|_{\underline{n} = \underline{n}_c} \qquad (80)$$

To deal with the first topological term, we add and subtract $\frac{\partial A^\alpha}{\partial n^\beta} \dot{n}_\beta \delta n^\alpha$, to get

$$\left. \begin{aligned} \delta \mathcal{S}_{Top} &= \delta \int_{t_1}^{t_2} d\tau\, \hbar S \underline{A} \cdot \dot{\underline{n}}(\tau) \Big|_{\underline{n} = \underline{n}_c} \\ &= \hbar S \int_{t_1}^{t_2} d\tau \Big\{ \Big[\frac{\partial A^\alpha}{\partial n^\beta} \delta n^\beta \dot{n}_\alpha - \frac{\partial A^\alpha}{\partial n^\beta} \delta n^\alpha \dot{n}_\beta \Big] \Big|_{\underline{n} = \underline{n}_c} \\ &\qquad + \Big[A^\alpha \frac{d}{dt} \delta n^\alpha + \frac{\partial A^\alpha}{\partial n^\beta} \dot{n}_\beta \delta n^\alpha \Big] \Big\} \\ &= \hbar S \int_{t_1}^{t_2} d\tau \Big[\epsilon^{\alpha\beta\gamma} \frac{\partial A^\alpha}{\partial n^\beta} (\dot{\underline{n}} \times \delta \underline{n})_\gamma + \frac{d}{dt} A^\alpha \delta n_\alpha \Big] \Big|_{\underline{n} = \underline{n}_c} \end{aligned} \right\} \qquad (81)$$

The 2nd term in this result is zero, since $\delta \underline{n} = 0$ at the 2 limiting points. We rewrite the 1st term using (58), and get a final result:

$$\delta \mathcal{S} = \int_{t_1}^{t_2} d\tau \left[\hbar S \, \epsilon^{\alpha\beta\gamma} n_\alpha \dot{n}_\beta - \frac{\partial \mathcal{H}}{\partial n_\gamma} \right]\Big|_{n=n_c} \delta n_\gamma \tag{82}$$

(note that from (58), $\underline{n}$ is parallel to $\dot{\underline{n}} \times \delta \underline{n}$). Eqtn. (82) then implies the eqtn. of motion

$$\dot{\underline{S}}_c(t) = \hbar S \dot{\underline{n}}_c(t) = \underline{n}_c \times \frac{\partial \mathcal{H}}{\partial \underline{n}_c} \tag{83}$$

This solution for $\underline{S}_c(t)$, in the semiclassical limit where $S \gg 1$, is exactly the same as the result given in (35). As with a classical particle, the basic idea here is that in the large S limit, interference between spin trajectories far from the classical path $\underline{n}_c(t)$ will be destructive, and that the kinetic term $\hbar S \underline{A} \cdot d\underline{n}$ oscillates rapidly with small changes $d\underline{n}$ away from $\underline{n}_c$, when S is large.

In the preceding discussion I have hardly scratched the surface of the topic of spin path integrals. Considerable discussion has raged over the correct form of the spin path integral, both in the semiclassical limit and otherwise; it is useful to look at some of the references in this context. The form we have given is designed to bring out the topological features of the system; but for practical applications many authors prefer to use the phase space formulation, and rewrite everything in terms of the complex coherent spin states $|z\rangle$, defined by

$$|z\rangle = \frac{1}{(1+\bar{z}z)^S} \, e^{z\hat{S}_-} |S,S\rangle \tag{84}$$

where the complex variable $z = \tan\theta/2 \, e^{i\varphi}$ (see Appendix). In this case the propagator takes the form

$$\left.\begin{aligned} G(z_2, z_1; t_2 t_1) &= \int_{\bar{z}_1}^{\bar{z}_2} \mathcal{D}\bar{\zeta}(\tau) \int_{z_1}^{z_2} \mathcal{D}\zeta(\tau) \, e^{i/\hbar \, \mathcal{S}[\bar{\zeta}, \zeta]} \\ \mathcal{S}[\bar{\zeta}, \zeta] &= \int_{t_1}^{t_2} d\tau \left[S\left(\frac{\dot{\bar{\zeta}}\zeta - \bar{\zeta}\dot{\zeta}}{1 + \bar{\zeta}\zeta} \right) - \mathcal{H}(\bar{\zeta}, \zeta) \right] \end{aligned}\right\} \tag{85}$$

The practical use of expressions like (61), (62), or (85) will become much clearer in the next section. They are particularly valuable in dealing with non-perturbative problems, such as the role of topology in spin dynamics, or in tunneling problems (which are inherently non-perturbative, since tunneling exponents $\sim \mathcal{S}/\hbar$).