Quantum magnetism of localized spins

We now move on to studying the many body physics of a more complicated system - a lattice of localized magnetic moments.

For concreteness, consider spin-S Heisenberg moments on some regular lattice with Hamiltonian

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + \ldots$$

... represents other interactions that might be present in any physical situation (Eg: terms that involve more than 2 spins, etc).

The interaction $\vec{S}_i \cdot \vec{S}_j$ is called the exchange interaction.

I will mainly discuss $J > 0$ (the antiferromagnetic case)

Various aspects of $J < 0$ (the ferromagnetic case) will be examined in a homework problem.

Origin of exchange in ~~electronic~~ insulators.

Consider electrons in a periodic solid described by the Hubbard model

$$H = -t \sum_{\substack{\langle ij \rangle \\ \alpha}} \left(c^{\dagger}_{i\alpha} c_{j\alpha} + h.c \right) + \frac{U}{2} \sum_i n_i (n_i - 1)$$

$$n_i = \sum_{\alpha} c^{\dagger}_{i\alpha} c_{i\alpha} = \text{total \# of electrons at site } i.$$

t - term hops electrons from each site to its nearest neighbours.

U = on-site repulsion between electrons that disfavors double occupancy on any site

(Longer range part of Coulomb interaction ignored in this model)

Consider situation in which there is 1 electron per site on average, i.e $\sum_i n_i = N$ where N = total # of sites.

Consider also the limit of large-U $\Rightarrow$ diagonalise H_U term first.

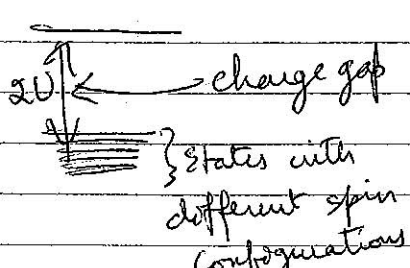
$$H_U = \frac{U}{2}\sum_i n_i(n_i - 1) \quad \Rightarrow \text{ Ground state has}$$

$n_i = 1 \;\; \forall$ sites but spin of electron is arbitrary.

$\therefore$ Gd state has 2^N-fold degeneracy.

Excited states (which preserve $\sum_i n_i = N$) correspond to removing a particle at one site & adding it to another site $\Rightarrow$ energy cost $2U$.

~~Ex~~ ~~Now~~ ~~Ex~~ Clearly system is an insulator in this limit as different sites do not even talk to each other



Now perturb by t.

For small $t \ll U$, expect

(a) Large ground state degeneracy (2^N) at $t = 0$ will be split.

(b) Charge gap will still stay finite, i.e.

excitations which correspond to taking a charge from one site & moving it to another will continue to cost finite energy

$\Rightarrow$ system will stay an insulator.

Note that insulating property is entirely a classical effect - coming from strong local Coulomb repulsion.

Such insulators are called Mott insulators.

[Many realizations in nature - various transition metal oxides, sulphides, etc : NiO, NiS, MnO, parent compounds of hiTc materials : La_2CuO_4, etc].

To describe splitting of 2^N-fold ground state manifold due to t, must do degenerate perturbation theory.

Goal: Find an effective Hamiltonian that lives in the Hilbert space of the ground state manifold that describes the low energy dynamics (at scales $\ll U$).

To 1^{st} order in t,

$$H_{eff} = P H_t P$$ where P projects onto gd state manifold

$$= 0 .$$

$\therefore$ Must go to 2^{nd} order in t.

To 2^{nd} order, from standard degenerate perturbation theory

$$\langle a | H_{eff} | b \rangle = \sum_A \frac{\langle a | H_t | A \rangle \langle A | H_t | b \rangle}{E_A - E_{gd}}$$

where $|a\rangle$, $|b\rangle$ are states in the ground state manifold

~~and~~ $|A\rangle$ refers to excited states outside the ground state manifold

$$\Rightarrow H_{eff} = \sum_A P \left(\frac{H_t | A \rangle \langle A | H_t}{E_A - E_{gd}} \right) P$$

Each term in H_t moves an electron from one site to a nearest neighbour.

$\therefore$ States $|A\rangle$ have one site that is empty & one of its nearest neighbours doubly occupied.

$\Rightarrow$ energy cost $E_A - E_{gd} = U$.

$$\therefore H_{eff} = -\frac{1}{U} P H_t^2 P$$

$$= -\frac{t^2}{U} \sum_{\substack{\langle ij \rangle \\ \langle kl \rangle}} P \left[\left(c_i^\dagger c_j + h.c \right) \left(c_k^\dagger c_l + h.c \right) \right] P$$

Only term that contributes is when the bond $\langle ij \rangle = \langle kl \rangle$.

$$\therefore H_{eff} = -\frac{t^2}{U} \sum_{\langle ij \rangle} P \left[\left(c_i^\dagger c_j + h.c \right)^2 \right] P$$

$$= -\frac{t^2}{U} \sum_{\langle ij \rangle} P \left[c_{i\alpha}^\dagger c_{j\alpha} c_{j\beta}^\dagger c_{i\beta} + c_{j\alpha}^\dagger c_{i\alpha} c_{i\beta}^\dagger c_{j\beta} \right] P$$

$$= -\frac{t^2}{U} \sum_{\langle ij \rangle} P \left[\left(c_{i\alpha}^\dagger c_{i\beta} \right) \left(c_{j\alpha} c_{j\beta}^\dagger \right) + \left(c_{j\alpha}^\dagger c_{j\beta} \right) \left(c_{i\alpha} c_{i\beta}^\dagger \right) \right] P$$

Write $c^\dagger_{i\alpha} c_{i\beta} = \vec{a}_i \cdot \vec{\sigma}_{\beta\alpha} + b_i \delta_{\beta\alpha}$

$$b_i = \tfrac{1}{2} c^\dagger_{i\alpha} \delta_{\alpha\beta} c_{i\beta} = \tfrac{1}{2} c^\dagger_i c_i = \tfrac{1}{2}$$

$$\vec{a}_i = \tfrac{1}{2} c^\dagger_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta} = \vec{S}_i = \text{spin on site } i.$$

$$\therefore c^\dagger_{i\alpha} c_{i\beta} = \vec{S}_i \cdot \vec{\sigma}_{\beta\alpha} + \tfrac{1}{2}\delta_{\beta\alpha}$$

$$c_{i\alpha} c^\dagger_{i\beta} = \delta_{\alpha\beta} - c^\dagger_{i\beta} c_{i\alpha}$$

$$= \tfrac{1}{2}\delta_{\alpha\beta} - \vec{S}_i \cdot \vec{\sigma}_{\alpha\beta}$$

$$\therefore H_{eff} = \frac{-t^2}{U} \sum_{\langle ij \rangle} \Big[\left(\vec{S}_i \cdot \vec{\sigma}_{\beta\alpha} + \tfrac{1}{2}\delta_{\beta\alpha}\right)\left(\tfrac{1}{2}\delta_{\alpha\beta} - \vec{S}_j \cdot \vec{\sigma}_{\alpha\beta}\right)$$

$$+ \left(\tfrac{1}{2}\delta_{\alpha\beta} - \vec{S}_i \cdot \vec{\sigma}_{\alpha\beta}\right)\left(\vec{S}_j \cdot \vec{\sigma}_{\beta\alpha} + \tfrac{1}{2}\delta_{\beta\alpha}\right)\Big]$$

$$= \frac{-t^2}{U} \sum_{\langle ij \rangle} \left[-4 \vec{S}_i \vec{S}_j + 1 \right]$$

$$= 4t^2/U \sum_{\langle ij \rangle} \left[\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \right].$$

$\Rightarrow$ At $o(t^2/U)$, get antiferromagnetic Heisenberg model of localized spin-$\frac{1}{2}$ moments with $J = 4t^2/U$.

At higher orders in the t/U expansion will get more complicated terms such as exchange along longer bonds or "multiparticle ring exchange" (which exchanges spins of 4 sites ~~de~~ on any elementary plaquette).

Here restrict to studying nearest neighbour model

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

$\vec{S}_i$ = spin-$\frac{1}{2}$ operators that satisfy

$$[S_i^a, S_j^b] = 0 \text{ if } i \neq j$$

$$[S_i^a, S_i^b] = i\epsilon^{abc} S_i^c .$$

Proceed as before for the Bose liquid - ~~...~~ make a semiclassical approximation.

First treat spins classically to find gd state, then ~~expand about~~ study small oscillations about classical ground state.

~~Approximation justified when size of S of spin $\rightarrow \infty$.~~

Each $S_i^a \sim o(S)$, but $[S_i^a, S_i^b]$ which involves products of 2 spins is also only of $o(S)$ rather than $o(S^2)$.

So semiclassical approximation can be systemized as an expansion of the physics in $1/S$.

0^{th} order in expansion: Classical limit

Succeeding orders: Quantum corrections.

~~$S \rightarrow \infty$ limit: If spins are classical, can ignore~~

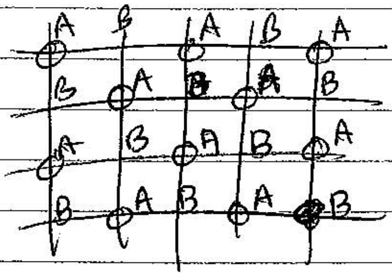
$\therefore$ Study more generally for arbitrary integer S.

$S \rightarrow \infty$: If spins are classical, can ignore their commutators.

Assume cubic lattice in d-dimensions.

$$H \text{ minimized when } \vec{S}_i = S\hat{z} \quad \text{if } i \in A$$
$$= -S\hat{z} \quad \text{if } i \in B$$

where A & B denote the 2 sublattices of the ~~sq~~ cubic lattice.



To understand the possible broken symmetry in the state, first examine the symmetries of the Heisenberg model.

$$H = J\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j \quad \text{is invariant under}$$

(i) All space group operations of the cubic lattice.

~~(ii) SU(2) rotation of all the spins:~~

$$\vec{S}_i \to U^{+}\vec{S}_i U$$

~~where $U = e^{i\vec{\alpha}\cdot\vec{\sigma}} \in SU(2)$~~

where U is an $SU(2)$ rotation

(For spin-$\frac{1}{2}$, $U = e^{i\vec{\alpha}\cdot\vec{\sigma}}$).

(iii) Time reversal $\mathcal{T}$:

$\mathcal{T}$ is an anti unitary transformation under which

$$\mathcal{T}\vec{S}_i\mathcal{T}^{-1} = -\vec{S}_i$$

$$\left(\text{Antiunitary} \Rightarrow \mathcal{T}(a\hat{O})\mathcal{T}^{-1} = a^* \mathcal{T}\hat{O}\mathcal{T}^{-1}\right).$$

The classical ground state $\vec{S}_i = \epsilon_i S\hat{z}$

with $\epsilon_i = +1$ on A, -1 on B clearly

breaks the full SU(2) spin rotation symmetry.

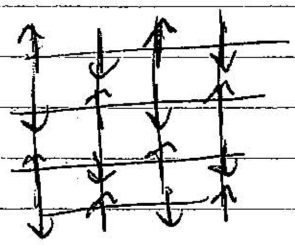
However rotations about $\hat{z}$ still remains unbroken

$\Rightarrow$ SU(2) is broken down to a U(1) subgroup of

rotations about the $\hat{z}$-axes of spin.

It also ~~appa~~ breaks symmetry of translation by one

lattice unit.



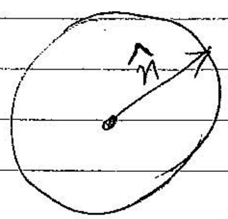
Time reversal is also apparently broken but

clearly combination of time reversal &

translation by one unit remains a good symmetry.

Based on this, we see that there clearly is a huge family of broken symmetry states related to each other by a global $SU(2)$ rotation.

In general any state $\vec{S}_i = \epsilon_i S \hat{n}$ with $\hat{n}$ an arbitrary unit vector is a classical ground state.



$\Rightarrow$ Manifold of classical ground states is the surface of a 2-sphere S^2.

$1/S$ - expansion (also known as spin-wave expansion).

... examine small harmonic fluctuations about classical gd state. (104)

This may be done systematically in a $1/S$ expansion.

Useful to define $S_i^{\pm} = S_{ix} \pm i S_{iy}$.

$$\left[S_i^{-}, S_i^{+} \right] = -2 S_{iz}$$

Consider expansion about any particular classical ground state, say $S_{iz} \simeq \epsilon_i S$ ($\epsilon_i = +1$ on A sublattice, -1 on B).

$\vec{S}_i$ satisfies $S_{iz}^2 + S_{ix}^2 + S_{iy}^2 = S_{iz}^2 + \frac{1}{2}\left(S_i^+ S_i^- + S_i^- S_i^+\right)$

$$= S(S+1).$$

To leading order in $1/S$, expect $S^{\pm}$ will have small matrix elements, so write

$$S_{iz} = \epsilon_i \sqrt{S(S+1) - \tfrac{1}{2}\left(S_i^+ S_i^- + S_i^- S_i^+\right)}$$

$$\simeq \epsilon_i S \left(1 + \frac{1}{2S} - \frac{1}{4S^2}\left(S_i^+ S_i^- + S_i^- S_i^+\right)\right).$$

In the commutation relation, can approximate $S_{iz} \simeq \epsilon_i S$

$$\Rightarrow \quad \left[S_i^-, S_i^+ \right] = -2\epsilon_i S.$$

This is almost the same commutation as for usual boson operators - only need to suitably normalize.

For $i \in A$, write $S_i^- = \sqrt{2S}\, a_i^+$, $S_i^+ = \sqrt{2S}\, a_i$

for $i \in B$, write $S_i^- = \sqrt{2S}\, a_i$, $S_i^+ = \sqrt{2S}\, a_i^+$

Then $[a_i, a_j^+] = \delta_{ij}$ so that a_i, a_i^+ are ~~the~~ usual boson operators.

$$S_{iz} = \epsilon_i\left(S + \tfrac{1}{2} - \frac{1}{2}\left(a_i^+ a_i + a_i a_i^+\right)\right)$$

$$= \epsilon_i\left(S - a_i^+ a_i\right)$$

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

~~For simplicity~~ Introduce ~~label~~ label $\vec{r}$ for sites on A

$\vec{r} + \hat{e}_\alpha$ $\left(\hat{e}_\alpha = \pm(\hat{e}_1, \hat{e}_2, \ldots \hat{e}_d)\right)$ are sites on B.

$$H = J \sum_{\vec{r}} \left(\sum_\alpha \vec{S}_r \cdot \vec{S}_{r+e_\alpha}\right)$$

$$= J \sum_{\vec{r}} \left(\sum_\alpha S_r^z S_{r+e_\alpha}^z + \tfrac{1}{2}\left(S_r^+ S_{r+e_\alpha}^- + h.c\right)\right)$$

$$= J \sum_{\vec{r}} \sum_\alpha \Big[-\left(S - a_r^+ a_r\right)\left(S - a_{r+\alpha}^+ a_{r+\alpha}\right)$$

$$+ S\left(a_r a_{r+\alpha} + h.c\right)\Big]$$

$$= \underbrace{-J d N S^2}_{\text{energy of classical gd state}} + JS \sum_{r} \sum_{\alpha} \underbrace{\left[a_r^\dagger a_r + a_{r+\alpha}^\dagger a_{r+\alpha} + a_r a_{r+\alpha} + h.c \right]}_{\text{Leading quantum correction}} + o(a^4)$$

The Hamiltonian (in this approximation) is quadratic in $(a, a^\dagger)$ & hence may be diagonalized easily.

Now notice that in terms of $(a_r, a_{r+\alpha}, \ldots)$ this quadratic Hamiltonian appears invariant under translation by one unit of the <u>original</u> cubic lattice

- so might as well simply state it as a problem on the original cubic lattice

$$\cancel{H_{quad}} \quad H_{SW} = JS \left[\sum_i 2d a_i^\dagger a_i + \sum_{\langle ij \rangle} (a_i a_j + h.c) \right]$$

Note however that relation of spin operators to $(a_i, a_i^\dagger)$ is different on A & B sublattices.

The 2d in the 1st term comes from the (2d) bonds that each spin participates in.

can now go to k-space

$$H_{SW} = JS \sum_{k} \left[2d\, a_k^{\dagger} a_k + \gamma_k \left(a_k a_{-k} + h.c \right) \right]$$

with $\gamma_k = 2 \sum_{n=1}^{d} \cos(k_n l)$

where l = lattice spacing.

From earlier calculation on such a Hamiltonian, we can read off excitation energies $E_k = JS \sqrt{4d^2 - \gamma_k^2}$

This vanishes when $\gamma_k = \pm 2d$ which happens for $k = 0$ (when $\gamma_k = +2d$) or when

$\vec{k} = \frac{1}{l}(\pi, \pi, \cdots, \pi)$ when $\gamma_k = -2d$.

Note that $\vec{k}$ is to be taken in 1st BZ of the cubic lattice

$\left(-\pi/l < k_n \leq \pi/l \right)$.

Thus there are 2 gapless points in $\vec{k}$-space $\Rightarrow$ there are 2 gapless modes.

Near either gapless $\vec{k}$ point if $\vec{q}$ represents deviation from it,

$$E_{\vec{q}} \approx JS \sqrt{4d^2 - 4d^2\left(1 - \frac{q^2}{2d}\right)} = \sqrt{2d}\, JS\, q$$

$\Rightarrow$ get linear dispersion ~~with~~ $E_k = ck$ with $c = \frac{JS\sqrt{2d}}{\cancel{\hbar}}$.

This mode will clearly determine the low-T thermodynamics of the antiferromagnet – these harmonic modes are known as spin waves or magnons.

Path-integral for spin

It will be very useful to develop a path-integral formulation of spin problems.

For a spin-S object, define spin coherent states $|\hat{n}\rangle$ through

$$\langle \hat{n} | \vec{S} | \hat{n} \rangle = S\hat{n}$$

$\Rightarrow$ $|\hat{n}\rangle = R(\hat{n})|\hat{z}\rangle$ with $R(\hat{n})$ the operator for a rotation of coordinate axes which puts $\hat{z}$-axis along $\hat{n}$.

Set of $|\hat{n}\rangle$ states are non-orthogonal & overcomplete.

In particular can resolve the identity in terms of these:

Consider the operator $\int \frac{d\hat{n}}{4\pi} (2S+1) |\hat{n}\rangle\langle\hat{n}|$

Clearly this is rotationally invariant

$$\Rightarrow \int \frac{d\hat{n}}{4\pi} (2S+1) |\hat{n}\rangle\langle\hat{n}| = \lambda \underline{1}$$

where $\underline{1}$ is the identity operator

Take the trace on both sides $\Rightarrow \lambda = 1$

$$\therefore \boxed{\underline{1} = \int \frac{d\hat{n}}{4\pi} (2S+1) |\hat{n}\rangle\langle\hat{n}|}$$

Consider a single spin degree of freedom with Hamiltonian $H = H(\vec{S})$.

Partition function $Z = \mathrm{Tr}\left(e^{-\beta H}\right)$

$$= (2S+1)\int \frac{d\hat{n}}{4\pi} \langle\hat{n}| e^{-\beta H} |\hat{n}\rangle$$

$$= (2S+1) \int \frac{d\hat{n}}{4\pi} \langle \hat{n} | \underbrace{e^{-\epsilon H} e^{-\epsilon H} \cdots e^{-\epsilon H}}_{N \text{ factors}} | \hat{n} \rangle$$

with $N\epsilon = \beta$.

$$= (2S+1)^N \int_{\hat{n}(N+1) = \hat{n}(N)} \left(\frac{d\hat{n}_1}{4\pi} \frac{d\hat{n}_2}{4\pi} \cdots \frac{d\hat{n}_N}{4\pi} \right)$$

$$\cancel{\langle \hat{n} |} \langle \hat{n}_{N+1} | e^{-\epsilon H} | \hat{n}_N \rangle$$

$$\cdots \langle \hat{n}_{j+1} | e^{-\epsilon H} | \hat{n}_j \rangle \cdots \langle \hat{n}_2 | e^{-\epsilon H} | \hat{n}_1 \rangle$$

$$\langle \hat{n}_{j+1} | e^{-\epsilon H} | \hat{n}_j \rangle \simeq \langle \hat{n}_{j+1} | 1 - \epsilon H | \hat{n}_j \rangle$$

$$= \langle \hat{n}_{j+1} | \hat{n}_j \rangle \left(1 - \epsilon \frac{\langle \hat{n}_{j+1} | H | \hat{n}_j \rangle}{\langle \hat{n}_{j+1} | \hat{n}_j \rangle} \right).$$

Assume

Assume that for the most important paths, to 0^{th} order in ϵ,

$$\frac{\langle \hat{n}_{j+1} | H | \hat{n}_j \rangle}{\langle \hat{n}_{j+1} | \hat{n}_j \rangle} \simeq \langle \hat{n}(\tau) | H | \hat{n}(\tau) \rangle = H(S\hat{n}(\tau)).$$

$$\left(\text{Notation: } j \to \tau = j\epsilon \right).$$

Write $|\hat{n}_{j+1}\rangle = |\hat{n}(\tau+\epsilon)\rangle \simeq |\hat{n}(\tau)\rangle + \epsilon \frac{d}{d\tau} |\hat{n}(\tau)\rangle$

to get

$$\langle \hat{n}(\tau+\epsilon) | e^{-\epsilon H} | \hat{n}(\tau) \rangle$$

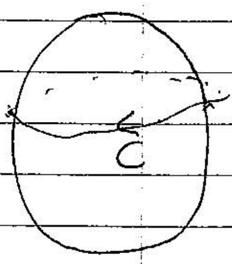
$$\simeq e^{-\epsilon \left[\langle \hat{n}(\tau) | \frac{d}{d\tau} | \hat{n}(\tau) \rangle + H(S\hat{n}(\tau)) \right]}$$

Then
$$Z = \int_{\hat{n}(\beta) = \hat{n}(0)} \left[D\hat{n}(\tau) \right] e^{-\int_0^\beta d\tau \left[\langle \hat{n}(\tau) | \frac{d}{d\tau} | \hat{n}(\tau) \rangle + H(S\hat{n}(\tau)) \right]}$$

$$\int \left[D\hat{n}(\tau) \right] = \lim_{\substack{\epsilon \to 0 \\ N \to \infty \\ N\epsilon = \beta}} \left[(2S+1)^N \prod_{j=1}^{N} \frac{d\hat{n}_j}{4\pi} \right]$$

The 1st term in the exponent

$$\int_0^\beta d\tau \left\langle \hat{n}(\tau) \right| \frac{d}{d\tau} \left| \hat{n}(\tau) \right\rangle \quad (= \text{Berry phase})$$



$$= \oint_C d\vec{s} \cdot \left\langle \hat{n}(\tau) \right| \frac{\partial}{\partial \hat{n}} \left| \hat{n}(\tau) \right\rangle$$

By Stokes theorem this closed line integral

$$= \int_{\substack{\text{area enclosed} \\ \text{by } C}} d\vec{A} \cdot \vec{\nabla} \times \left\langle \hat{n} \right| \nabla_{\hat{n}} \left| \hat{n} \right\rangle$$

$$\equiv \int d\vec{A} \cdot \vec{\mathcal{B}}$$

with $\mathcal{B}_i = \epsilon_{ijk} \partial_j \left\langle \hat{n} \right| \partial_k \left| \hat{n} \right\rangle$

where derivatives $\partial_j = \dfrac{\partial}{\partial n_j}$.

Note: View $\hat{n}$-sphere as embedded in R^3, i.e. assume $n_{x,y,z}$ can vary independently at first, then restrict loop C to lie on unit sphere at end of calculation.

Introduce complete set of states $|\hat{n}_m(r)\rangle$ which are eigenstates of $\vec{S}\cdot\hat{n}(r)$.

Clearly $|\hat{n}(r)\rangle = |\hat{n}_s(r)\rangle$

Consider $\langle n_m | (\vec{S}\cdot\hat{n}) | n_{m'}\rangle = m\,\delta_{mm'}$.

For $m \neq m'$, differentiate w.r.t n_k

$$\Big(\partial_k \langle n_m|\Big)\Big(m'\,|n_{m'}\rangle\Big) + \langle n_m| S_k |n_{m'}\rangle$$

$$+ \Big(\langle n_m|\,m\Big)\,\partial_k |n_{m'}\rangle = 0 .$$

$$\Rightarrow\; m'\Big(\partial_k \langle n_m|\Big)|n_{m'}\rangle + m\,\langle n_m|\partial_k|n_{m'}\rangle$$

$$+ \langle n_m| S_k |n_{m'}\rangle$$

$$= 0 .$$

(Reminder: n_x, n_y, n_z are independent variables at this stage – so $\dfrac{\partial n_\ell}{\partial n_k} = \delta_{\ell k}$; at end of calculation will only consider $\hat{n}$-trajectories that lie on unit sphere).

Now use $\langle m|m'\rangle = 0$ (for $m \neq m'$) to write

$$\left(\partial_k \langle m|\right)|m'\rangle = -\langle m|\partial_k|m'\rangle$$

$$\therefore \quad \langle m|\partial_k|m'\rangle = \frac{\langle m|S_k|m'\rangle}{m'-m} \quad \text{for } m\neq m'.$$

$$B_i = \epsilon_{ijk}\,\partial_j \langle \hat{n}_s|\partial_k|\hat{n}_s\rangle$$

$$= \frac{1}{2}\epsilon_{ijk}\left(\partial_j\langle \hat{n}_s|\partial_k|\hat{n}_s\rangle - \partial_k\langle \hat{n}_s|\partial_j|\hat{n}_s\rangle\right)$$

$$= \frac{1}{2}\epsilon_{ijk}\sum_m \Big(\left(\partial_j\langle \hat{n}_s|\right)|\hat{n}_m\rangle\langle \hat{n}_m|\partial_k|\hat{n}_s\rangle$$

$$- \left(\partial_k\langle \hat{n}_s|\right)|\hat{n}_m\rangle\langle \hat{n}_m|\partial_j|\hat{n}_s\rangle$$

$$+ \langle \hat{n}_s|\partial_j\partial_k - \partial_k\partial_k|\hat{n}_s\rangle\Big)$$

$$= \frac{1}{2}\epsilon_{ijk}\sum_{m\neq s} \langle \hat{n}_s|\partial_k|\hat{n}_m\rangle\langle \hat{n}_m|\partial_j|\hat{n}_s\rangle - \langle \hat{n}_s|\partial_j|\hat{n}_m\rangle\langle \hat{n}_m|\partial_k|\hat{n}_s\rangle$$

Comments / clarifications.

To make sure there is no confusion, let us consider various points

(i) Specialize to spin $\frac{1}{2}$.

Then the wave function of any state is a spinor.

Eg: $|\hat{z}\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

Let the spinor wave function of the coherent state $|\hat{n}\rangle$ be $z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$ with $z^\dagger z = |z_1|^2 + |z_2|^2 = 1$.

$$\langle \hat{n} | \vec{S} | \hat{n} \rangle = S\hat{n} \Rightarrow z^\dagger \vec{\sigma} z = \hat{n}.$$

If $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$,

then can choose
$$z = e^{i\phi/2} \begin{bmatrix} e^{i\phi/2} \cos\theta/2 \\ e^{-i\phi/2} \sin\theta/2 \end{bmatrix}$$

$$= \begin{bmatrix} e^{i\phi} \cos\frac{\theta}{2} \\ \sin\theta/2 \end{bmatrix}$$

This wave function is single-valued on the $\hat{n}$-sphere.

In the path integral, the "Berry phase" term is

$$\int_0^\beta d\tau \left\langle \hat{n}(\tau) \right| \frac{d}{d\tau} \left| \hat{n}(\tau) \right\rangle$$

$$= \int_0^\beta d\tau \; z^\dagger \frac{d}{d\tau} z .$$

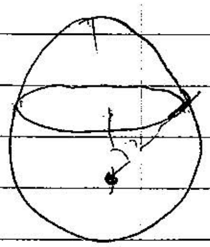
$$\frac{dz}{d\tau} = \begin{bmatrix} i \frac{d\phi}{d\tau} e^{i\phi} \cos\frac{\theta}{2} - \frac{1 \, d\theta}{2 d\tau} e^{i\phi} \sin\frac{\theta}{2} \\ \left(\frac{1}{2}\frac{d\theta}{d\tau}\right) \cos\theta/2 \end{bmatrix} .$$

$$\therefore z^\dagger \frac{dz}{d\tau} = i\left(\frac{d\phi}{d\tau}\right)\cos^2\frac{\theta}{2} \cancel{- \frac{1}{2}\frac{d\theta}{d\tau} \cos\frac{\theta}{2} \sin\theta/2}$$

$$\cancel{+ \tfrac{1}{2}\frac{d\theta}{d\tau}\cos\theta/2 \, \sin\theta/2}$$

$$= i\left(\frac{d\phi}{d\tau}\right)\left(\frac{1-\cos\theta}{2}\right) .$$

$$\int_0^\beta d\tau \; z^\dagger \frac{dz}{d\tau} = i \int_0^\beta d\tau \left(\frac{d\phi}{d\tau}\right)\left(\frac{1-\cos\theta}{2}\right).$$



$$= \left(\frac{i}{2}\right) \oint_C (d\phi)\,(1-\cos\theta).$$

Now use $1-\cos\theta = \int_0^\theta d\theta' \sin\theta'$

$$\therefore \int_0^\beta d\tau \; z^\dagger \frac{dz}{d\tau} = \frac{i}{2} \oint_C d\phi \int_0^\theta d\theta' \sin\theta'$$

$$= \frac{i}{2} \int_{\substack{\text{area bounded}\\ \text{by } C}} d\phi \, d\theta' \sin\theta'$$

$$= \frac{i}{2} \int_{\substack{\text{area bounded}\\ \text{by } C}} d\Omega$$

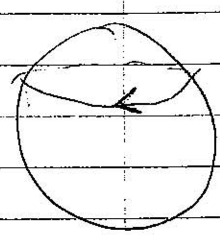
$$= \frac{i}{2}\left(\text{solid angle of cap on sphere bounded by } C\right)$$

which is the same result as before (specializing to spin-$\frac{1}{2}$)

(ii) Can therefore rewrite this term as

$$iS \int_0^\beta d\tau \; \vec{A}(\hat{n}) \cdot \frac{d\hat{n}}{d\tau}$$

where $\vec{A}(\hat{n})$ is the vector potential of a magnetic monopole of unit strength at the origin of the $\hat{n}$-sphere.



Note: whether we take area of upper cap or lower cap makes no difference.

$$A_{upper} = 4\pi + A_{lower}$$

$$\Rightarrow e^{iS A_{upper}} = e^{4\pi i S} \, e^{iS A_{lower}}$$

But $e^{4\pi i S} = 1$ as $S = 0, \frac{1}{2}, 1, \ldots$ so get the same answer.

(iii) Earlier derivation is concise but perhaps a bit slick. To proceed more carefully introduce some coordinates (x_1, x_2) on the surface of the sphere

Eg: $(x_1, x_2) = (\theta, \phi)$.

$$z = z(x_1, x_2).$$

$$z^\dagger \frac{dz}{d\sigma} = \left(z^\dagger \partial_1 z\right)\dot{x}_1 + \left(z^\dagger \partial_2 z\right)\dot{x}_2$$

$$\int_0^\beta d\sigma \; z^\dagger \frac{dz}{d\sigma} = \oint_C d\vec{x} \cdot z^\dagger \vec{\nabla} z$$

$$= \int d\vec{A} \cdot \vec{\nabla} \times \left(z^\dagger \vec{\nabla} z\right)$$

$$= \int d\vec{A} \cdot \vec{\nabla} z^\dagger \times \vec{\nabla} z = \int d\vec{A} \cdot \vec{B}$$

$$\left(dA = dx_1\, dx_2\right)$$

$$\vec{B} = \left(\vec{\nabla} z^\dagger\right) \times \left(z z^\dagger + w w^\dagger\right) \vec{\nabla} z = \left(\left(\nabla z^\dagger\right) w\right) \times \left(w^\dagger \nabla z\right)$$

$$= -\left(z^\dagger \nabla w\right) \times \left(w^\dagger \nabla z\right).$$

~~Consider~~ $\cancel{z^\dagger(\vec{\sigma}\cdot\hat{n}) w = 0}$ ~~for~~ where $w = \left(-i\sigma_y\right)\left(z^\dagger\right)^T$

is the eigenspinor with eigenvalue -1 of $\vec{\sigma}\cdot\hat{n}$.

$$z^\dagger\left(\vec{\sigma}\cdot\hat{n}\right) w = 0 \Rightarrow 2 z^\dagger \vec{\nabla} w + z^\dagger\left(\vec{\sigma}\cdot\vec{\nabla}\hat{n}\right) w = 0$$

$$\Rightarrow z^\dagger \partial_i w = -\frac{1}{2} z^\dagger \left(\vec{\sigma}\cdot\partial_i \hat{n}\right) w$$

Similarly $w^\dagger \partial_i z = +\frac{1}{2} w^\dagger \left(\vec{\sigma}\cdot\partial_i\hat{n}\right) z.$

$$\Rightarrow \mathcal{B}_i = \frac{+}{4}\epsilon_{ijk}\left(z^\dagger \sigma^a \partial_i n^a\, w\right)\left(w^\dagger \sigma^b \partial_j n^b\, z\right)$$

$$= \frac{\epsilon_{ijk}}{4} z^\dagger \left(\sigma^a \sigma^b \partial_i n^a \partial_j n^b\right) z$$

$$= \frac{i}{2}\epsilon_{ijk}\epsilon^{abc}\left(\partial_i n^a \partial_j n^b\right)\left(z^\dagger \sigma^c z\right)$$

$$= \frac{i}{2}\epsilon_{ijk}\left(\partial_i n^a \partial_j n^b n^c\right)\left(\epsilon^{abc}\right)$$

$$= \frac{i}{2}\epsilon_{ijk}\, \hat{n} \cdot \partial_i \hat{n} \times \partial_j \hat{n} .$$

$\int \mathcal{B}_i \, dA_i = {}^{i}/_{2}$ (area on surface of sphere bounded by C).

($\hat{n} = \hat{n}(x_1, x_2)$ is a map from (x_1, x_2) to surface of sphere ; $\epsilon_{ijk}\hat{n} \cdot \partial_i \hat{n} \times \partial_j \hat{n}\; dx_1 dx_2$ = area on sphere corresponding to area $dx_1 dx_2$) .

$$= -\tfrac{1}{2}\,\epsilon_{ijk} \sum_{m \neq s} \frac{\left[\langle \hat{n}_s | S_k | \hat{n}_m \rangle \langle \hat{n}_m | S_j | \hat{n}_s \rangle - \langle \hat{n}_s | S_j | \hat{n}_m \rangle \langle \hat{n}_m | S_k | \hat{n}_s \rangle\right]}{(m-s)^2}$$

Matrix elements are non-zero only if $m = s \pm 1$

$$\Rightarrow \mathcal{B}_i = \tfrac{1}{2}\,\epsilon_{ijk} \sum_m \Big(\langle \hat{n}_s | S_j | \hat{n}_m \rangle \langle \hat{n}_m | S_k | \hat{n}_s \rangle - \langle \hat{n}_s | S_k | \hat{n}_m \rangle \langle \hat{n}_m | S_j | \hat{n}_s \rangle \Big)$$

$$= \tfrac{1}{2}\,\epsilon_{ijk} \langle \hat{n}_s | [S_j, S_k] | \hat{n}_s \rangle$$

$$= \tfrac{i}{2}\,\epsilon_{ijk}\,\epsilon_{jkl} \langle \hat{n}_s | S_l | \hat{n}_s \rangle$$

$$= \frac{iS}{2}\,\epsilon_{ijk}\,\epsilon_{jkl}\, n_l = iS\,\hat{n}_i$$

$$\therefore \vec{\mathcal{B}} = iS\,\hat{n}$$

$$\therefore \int_0^\beta d\tau \, \langle \hat{n} | \frac{d}{d\tau} | \hat{n} \rangle = i\,(\text{flux of } \mathcal{B} \text{ thru } C)$$

$$= iS\,(\text{area swept by string connecting north pole to } \hat{n}(\tau))$$

$$= (iS) \int_0^1 du \int_0^\beta d\tau \; \hat{n}(\tau, u) \cdot \left(\partial_\tau \hat{n} \times \partial_u \hat{n} \right)$$

$u \in [0, 1]$ = parameter along arc of great circle connecting north pole to $\hat{n}(\tau)$ such that

$\hat{n}(u=0) = \hat{z}$, and $\hat{n}(u=1) = \hat{n}(\tau)$.

$$\therefore \; Z = \int [\mathcal{D}\hat{n}] \; e^{-\left(iS \underbrace{\mathcal{A}[\hat{n}(\tau)]}_{\text{area of loop as above}} + \int_0^\beta d\tau \, H(S\hat{n}(\tau)) \right)}$$

For a system of many interacting spins at sites labelled by i & a Hamiltonian depending linearly on each spin variable

$$Z = \int \prod_i [\mathcal{D}\hat{n}_i] \; e^{-\left[iS \sum_i \mathcal{A}_i[\hat{n}_i(\tau)] + \int_0^\beta d\tau \, H(\{S\hat{n}_i(\tau)\}) \right]}.$$