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# Chapter 15

## Spins, Coherent States, Path Integrals, and Applications

### 15.1 The Coherent State Path Integral

#### 15.1.1 Feynman path integral

The path integral formulation of quantum mechanics is both beautiful and powerful. It is useful in elucidating the quantum-classical correspondence and the semiclassical approximation, in accounting for interference effects, in treatments of tunneling problems via the method of instantons, *etc.* Our goal is to derive and to apply a path integral method for quantum spin. We begin by briefly reviewing the derivation of the usual Feynman path integral.

Consider the propagator  $K(x_i, x_f, T)$ , which is the probability amplitude that a particle located at  $x = x_i$  at time  $t = 0$  will be located at  $x = x_f$  at time  $t = T$ . We may write

$$\begin{aligned} K(x_i, x_f, T) &= \langle x_f | e^{-iHT/\hbar} | x_i \rangle \\ &= \langle x_N | e^{-i\epsilon H/\hbar} 1 e^{-i\epsilon H/\hbar} 1 \dots 1 e^{-i\epsilon H/\hbar} | x_0 \rangle \end{aligned} \quad (15.1)$$

where  $\epsilon = T/N$ , and where we have defined  $x_0 \equiv x_i$  and  $x_N \equiv x_f$ . We are interested in the limit  $N \rightarrow \infty$ . Inserting  $(N - 1)$  resolutions of the identity of the form

$$1 = \int_{-\infty}^{\infty} dx_j |x_j\rangle \langle x_j|, \quad (15.2)$$

we find that we must evaluate matrix elements of the form

$$\begin{aligned}
 \langle x_{j+1} | e^{-iH\epsilon/\hbar} | x_j \rangle &\approx \int_{-\infty}^{\infty} dp_j \langle x_{j+1} | p_j \rangle \langle p_j | e^{-iT\epsilon/\hbar} e^{-iV\epsilon/\hbar} | x_j \rangle \\
 &= \int_{-\infty}^{\infty} dp_j e^{ip_j(x_{j+1}-x_j)} e^{-i\epsilon p_j^2/2m\hbar} e^{-i\epsilon V(x_j)/\hbar} .
 \end{aligned} \tag{15.3}$$

The propagator may now be written as

$$\begin{aligned}
 \langle x_N | e^{-iHT/\hbar} | x_0 \rangle &\approx \int_{-\infty}^{\infty} \prod_{j=1}^{N-1} dx_j \int_{-\infty}^{\infty} \prod_{k=0}^{N-1} dp_k \exp \left\{ i \sum_{k=0}^{N-1} \left[ p_k(x_{k+1} - x_k) - \frac{\epsilon}{2m\hbar} p_k^2 - \frac{\epsilon}{\hbar} V(x_k) \right] \right\} \\
 &= \left( \frac{2\pi\hbar m}{i\epsilon} \right)^N \int_{-\infty}^{\infty} \prod_{j=1}^{N-1} dx_j \exp \left\{ \frac{i\epsilon}{\hbar} \sum_{k=1}^{N-1} \left[ \frac{1}{2} m \left( \frac{x_{j+1} - x_j}{\epsilon} \right)^2 - V(x_j) \right] \right\} \\
 &\equiv \int_{\substack{x(0)=x_i \\ x(T)=x_f}} \mathcal{D}x(t) \exp \left\{ \frac{i}{\hbar} \int_0^T dt \left[ \frac{1}{2} m \dot{x}^2 - V(x) \right] \right\} ,
 \end{aligned} \tag{15.4}$$

where we absorb the prefactor into the measure  $\mathcal{D}x(t)$ . Note the boundary conditions on the path integral at  $t = 0$  and  $t = T$ . In the semiclassical approximation, we assume that the path integral is dominated by trajectories  $x(t)$  which extremize the argument of the exponential in the last term above. This quantity is (somewhat incorrectly) identified as the classical action,  $\mathcal{S}$ , and the action-extremizing equations are of course the Euler-Lagrange equations. Setting  $\delta\mathcal{S} = 0$  yields Newton's second law,  $m\ddot{x} = -\partial V/\partial x$ , which is to be solved subject to the two boundary conditions.

The 'imaginary time' version, which yields the 'thermal propagator', is obtained by writing  $T = -i\hbar\beta$  and  $t = -i\tau$ , in which case

$$\langle x_f | e^{-\beta H} | x_i \rangle = \int_{\substack{x(0)=x_i \\ x(\hbar\beta)=x_f}} \mathcal{D}x(\tau) \exp \left\{ - \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left[ \frac{1}{2} m \dot{x}^2 + V(x) \right] \right\} . \tag{15.5}$$

'Euclidean action'  $\mathcal{S}_E$

The partition function is the trace of the thermal propagator, *viz.*

$$Z = \text{Tr} e^{-\beta H} = \int_{-\infty}^{\infty} dx \langle x | e^{-\beta H} | x \rangle = \int_{x(0)=x(\hbar\beta)} \mathcal{D}x(\tau) \exp(-\mathcal{S}_E[x(\tau)]/\hbar) \tag{15.6}$$

The equations of motion derived from  $\mathcal{S}_E$  are  $m\ddot{x} = +\partial V/\partial x$ , corresponding to motion in the ‘inverted potential’.

### 15.1.2 Coherent state path integral for the ‘Heisenberg-Weyl’ hroup

We now turn to the method of coherent state path integration. In order to discuss this, we must first introduce the notion of coherent states. This is most simply done by appealing to the one-dimensional simple harmonic oscillator,

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 = \hbar\omega_0 \left( a^\dagger a + \frac{1}{2} \right) , \quad (15.7)$$

where  $a$  and  $a^\dagger$  are ladder operators,

$$a = \ell \partial_x + \frac{x}{2\ell} , \quad a^\dagger = -\ell \partial_x + \frac{x}{2\ell} \quad (15.8)$$

with  $\ell \equiv \sqrt{\hbar/2m\omega_0}$ . *Exercise: Check that  $[a, a^\dagger] = 1$ .*

The ground state satisfies  $a\psi_0(x) = 0$ , which yields

$$\psi_0(x) = (2\pi\ell^2)^{-1/4} \exp(-x^2/4\ell^2) . \quad (15.9)$$

The normalized coherent state  $|z\rangle$  is defined as

$$|z\rangle = e^{-\frac{1}{2}|z|^2} e^{za^\dagger} |0\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle . \quad (15.10)$$

The coherent state is an eigenstate of the annihilation operator  $a$ :

$$a|z\rangle = z|z\rangle \quad \Longleftrightarrow \quad \langle z|a^\dagger = \langle z|\bar{z} . \quad (15.11)$$

The overlap of coherent states is given by

$$\langle z_1 | z_2 \rangle = e^{-\frac{1}{2}|z_1|^2} e^{-\frac{1}{2}|z_2|^2} e^{\bar{z}_1 z_2} , \quad (15.12)$$

hence different coherent states are not orthogonal. Despite this nonorthogonality, the coherent states allow a simple resolution of the identity,

$$1 = \int \frac{d^2z}{2\pi i} |z\rangle\langle z| , \quad \frac{d^2z}{2\pi i} \equiv \frac{d\operatorname{Re}z d\operatorname{Im}z}{\pi} \quad (15.13)$$

which is straightforward to establish.

To gain some physical intuition about the coherent states, define

$$z \equiv \frac{Q}{2\ell} + \frac{i\ell P}{\hbar} . \quad (15.14)$$

One finds (*exercise!*)

$$\psi_{P,Q}(x) = \langle x | z \rangle = (2\pi\ell^2)^{-1/4} e^{-iPQ/2\hbar} e^{iPx/\hbar} e^{-(x-Q)^2/4\ell^2} , \quad (15.15)$$

hence the coherent state  $\psi_{P,Q}(x)$  is a wavepacket Gaussianly localized about  $x = Q$ , but oscillating with momentum  $P$ . *Exercise: Compute*  $\langle (q - Q)^2 \rangle$  *and*  $\langle (p - P)^2 \rangle$ .

Now we derive the imaginary time path integral. We write

$$\langle z_f | e^{-\beta H} | z_i \rangle = \langle z_N | e^{-\epsilon H/\hbar} 1 e^{-\epsilon H/\hbar} \dots 1 e^{-\epsilon H/\hbar} | z_0 \rangle , \quad (15.16)$$

inserting resolutions of the identity at  $N - 1$  points, as before. We next evaluate the matrix element

$$\begin{aligned} \langle z_j | e^{-\epsilon H/\hbar} | z_{j-1} \rangle &= \langle z_j | z_{j-1} \rangle \cdot \left\{ 1 - \frac{\epsilon}{\hbar} \frac{\langle z_j | H | z_{j-1} \rangle}{\langle z_j | z_{j-1} \rangle} + \dots \right\} \\ &\simeq \langle z_j | z_{j-1} \rangle \exp \left\{ -\frac{\epsilon}{\hbar} H(\bar{z}_j | z_{j-1}) \right\} \end{aligned} \quad (15.17)$$

where

$$H(\bar{z}|w) \equiv \frac{\langle z | H | w \rangle}{\langle z | w \rangle} = e^{-\bar{z}w} \langle 0 | e^{\bar{z}a} H(a^\dagger, a) e^{wa^\dagger} | 0 \rangle . \quad (15.18)$$

This last equation is extremely handy. It says, upon invoking eqn. 15.11, that if  $H(a, a^\dagger)$  is *normal ordered* such that all creation operators  $a^\dagger$  appear to the *left* of all destruction operators  $a$ , then  $H(\bar{z}|w)$  is obtained from  $H(a^\dagger, a)$  simply by sending  $a^\dagger \rightarrow \bar{z}$  and  $a \rightarrow w$ . This is because  $a$  acting to the right on  $|w\rangle$  yields its eigenvalue  $w$ , while  $a^\dagger$  acting to the left on  $\langle z|$  generates  $\bar{z}$ . Note that the function  $H(\bar{z}|w)$  is holomorphic in  $w$  and in  $\bar{z}$ , but is completely independent of their complex conjugates  $\bar{w}$  and  $z$ .

The overlap between coherent states at consecutive time slices may be written

$$\langle z_j | z_{j-1} \rangle = \exp \left\{ -\frac{1}{2} \left[ \bar{z}_j (z_j - z_{j-1}) - z_{j-1} (\bar{z}_j - \bar{z}_{j-1}) \right] \right\} , \quad (15.19)$$

hence

$$\begin{aligned} \langle z_N | z_{N-1} \rangle \dots \langle z_1 | z_0 \rangle &= \exp \left\{ \frac{1}{2} \sum_{j=1}^{N-1} \left[ z_j (\bar{z}_{j+1} - \bar{z}_j) - \bar{z}_j (z_j - z_{j-1}) \right] \right\} \\ &\quad \times \exp \left\{ \frac{1}{2} z_0 (\bar{z}_1 - \bar{z}_0) - \frac{1}{2} \bar{z}_N (z_N - z_{N-1}) \right\} , \end{aligned} \quad (15.20)$$



which allows us to write down the path integral expression for the propagator,

$$\begin{aligned} \langle z_f | e^{-\beta H} | z_i \rangle &= \int \prod_{j=1}^{N-1} \frac{d^2 z_j}{2\pi i} \exp \left( -\mathcal{S}_E[\{z_j, \bar{z}_j\}]/\hbar \right) \\ \mathcal{S}_E[\{z_j, \bar{z}_j\}]/\hbar &= \sum_{j=1}^{N-1} \left[ \frac{1}{2} \bar{z}_j (z_j - z_{j-1}) - \frac{1}{2} z_j (\bar{z}_{j+1} - \bar{z}_j) \right] + \frac{\epsilon}{\hbar} \sum_{j=1}^N H(\bar{z}_j | z_{j-1}) \\ &\quad + \frac{1}{2} \bar{z}_f (z_f - z_{N-1}) - \frac{1}{2} z_i (\bar{z}_1 - \bar{z}_i) \quad . \end{aligned} \quad (15.21)$$

In the limit  $N \rightarrow \infty$ , we identify the continuum Euclidean action

$$\begin{aligned} \mathcal{S}_E[\{z(\tau), \bar{z}(\tau)\}]/\hbar &= \int_0^{\hbar\beta} d\tau \left\{ \frac{1}{2} \left( \bar{z} \frac{\partial z}{\partial \tau} - z \frac{\partial \bar{z}}{\partial \tau} \right) + \frac{1}{\hbar} H(\bar{z}|z) \right\} \\ &\quad + \frac{1}{2} \bar{z}_f [z_f - z(\hbar\beta)] - \frac{1}{2} z_i [\bar{z}(0) - \bar{z}_i] \quad , \end{aligned} \quad (15.22)$$

and write the continuum expression for the path integral,

$$\langle z_f | e^{-\beta H} | z_i \rangle = \int \mathcal{D}[z(\tau), \bar{z}(\tau)] e^{-\mathcal{S}_E[\{z(\tau), \bar{z}(\tau)\}]/\hbar} \quad . \quad (15.23)$$

The continuum limit is in a sense justified by examining the discrete equations of motion,

$$\begin{aligned} \frac{1}{\hbar} \frac{\partial \mathcal{S}_E}{\partial z_k} &= \bar{z}_k - \bar{z}_{k+1} + \frac{\epsilon}{\hbar} \frac{\partial H(\bar{z}_{k+1}|z_k)}{\partial z_k} \\ \frac{1}{\hbar} \frac{\partial \mathcal{S}_E}{\partial \bar{z}_k} &= z_k - z_{k-1} + \frac{\epsilon}{\hbar} \frac{\partial H(\bar{z}_k|z_{k-1})}{\partial \bar{z}_k} \quad , \end{aligned} \quad (15.24)$$

which have the sensible continuum limit

$$\hbar \frac{\partial \bar{z}}{\partial \tau} = \frac{\partial H(\bar{z}|z)}{\partial z} \quad , \quad \hbar \frac{\partial z}{\partial \tau} = -\frac{\partial H(\bar{z}|z)}{\partial \bar{z}} \quad (15.25)$$

with boundary conditions  $\bar{z}(\hbar\beta) = \bar{z}_f$  and  $z(0) = z_i$ . Note that there are only two boundary conditions – one on  $z(0)$  and the other on  $\bar{z}(\hbar\beta)$ . The function  $z(\tau)$  (or its discrete version  $z_j$ ) is evolved forward from initial data  $z_i$ , while  $\bar{z}(\tau)$  (or  $\bar{z}_j$ ) is evolved backward from final data  $\bar{z}_f$ . This is the proper number of boundary conditions to place on two first order differential (or finite difference) equations. It is noteworthy that the action of eqn. 15.21 or eqn. 15.22 imposes only a *finite* penalty on *discontinuous* paths.<sup>1</sup> Nevertheless, the paths which extremize the action are continuous throughout the interval  $\tau \in (0, \hbar\beta)$ . As  $z(\tau)$  is integrated forward from  $z_i$ , its

<sup>1</sup>In the Feynman path integral, discontinuous paths contribute an infinite amount to the action, and are therefore suppressed.

final value  $z(\hbar\beta)$  will in general be different from  $z_f$ . Similarly,  $\bar{z}(\tau)$  integrated backward from  $\bar{z}_f$  will in general yield an endpoint value  $\bar{z}(0)$  which differs from  $\bar{z}_i$ . The differences  $z(\hbar\beta) - z_f$  and  $\bar{z}(0) - \bar{z}_i$  are often identified as path discontinuities, but the fact is that the equations of motion know nothing about either  $z_f$  or  $\bar{z}_i$ . These difference terms do enter in a careful accounting of the action formulae of eqns. 15.21 and 15.22, however.

The importance of the boundary terms is nicely illustrated in a computation of the semiclassical imaginary time propagator for the harmonic oscillator. With  $H = \hbar\omega_0 a^\dagger a$  (dropping the constant term for convenience), we have

$$\begin{aligned} \langle z_f | \exp(-\beta\hbar\omega_0 a^\dagger a) | z_i \rangle &= e^{-\frac{1}{2}|z_f|^2 - \frac{1}{2}|z_i|^2} \sum_{m,n=0}^{\infty} \frac{\bar{z}_f^m z_i^n}{\sqrt{m!n!}} \langle m | \exp(-\beta\hbar\omega_0 a^\dagger a) | n \rangle \\ &= \exp \left\{ -\frac{1}{2}|z_f|^2 - \frac{1}{2}|z_i|^2 + \bar{z}_f z_i e^{-\beta\hbar\omega_0} \right\} . \end{aligned} \quad (15.26)$$

The Euclidean action is  $L_E = \frac{1}{2}\hbar(\bar{z}\dot{z} - z\dot{\bar{z}}) + \hbar\omega_0 \bar{z}z$ , so the equations of motion are

$$\hbar\dot{\bar{z}} = \frac{\partial H}{\partial z} = \hbar\omega_0 \bar{z} \quad , \quad \hbar\dot{z} = -\frac{\partial H}{\partial \bar{z}} = -\hbar\omega_0 z \quad (15.27)$$

subject to boundary conditions  $z(0) = z_i$ ,  $\bar{z}(\hbar\beta) = \bar{z}_f$ . The solution is

$$z(\tau) = z_i e^{-\omega_0\tau} \quad , \quad \bar{z}(\tau) = \bar{z}_f e^{\omega_0(\tau-\hbar\beta)} . \quad (15.28)$$

Along the ‘classical path’ the Euclidean Lagrangian vanishes:  $L_E = 0$ . The entire contribution to the action therefore comes from the boundary terms:

$$\begin{aligned} \mathcal{S}_E^{\text{cl}}/\hbar &= 0 + \frac{1}{2}\bar{z}_f(z_f - z_i e^{-\beta\hbar\omega_0}) - \frac{1}{2}z_i(\bar{z}_f e^{-\beta\hbar\omega_0} - \bar{z}_i) \\ &= \frac{1}{2}|z_f|^2 + \frac{1}{2}|z_i|^2 - \bar{z}_f z_i e^{-\beta\hbar\omega_0} \quad , \end{aligned} \quad (15.29)$$

What remains is to compute the fluctuation determinant. We write

$$z_j = z_j^{\text{cl}} + \eta_j \quad , \quad \bar{z}_j = \bar{z}_j^{\text{cl}} + \bar{\eta}_j \quad , \quad (15.30)$$

and expand the action as

$$\begin{aligned} \mathcal{S}_E[\{z_j, \bar{z}_j\}] &= \mathcal{S}_E[\{z_j^{\text{cl}}, \bar{z}_j^{\text{cl}}\}] + \frac{\partial^2 \mathcal{S}_E}{\partial \bar{z}_i \partial z_j} \bar{\eta}_i \eta_j + \frac{1}{2} \frac{\partial^2 \mathcal{S}_E}{\partial z_i \partial z_j} \eta_i \eta_j + \frac{1}{2} \frac{\partial^2 \mathcal{S}_E}{\partial \bar{z}_i \partial \bar{z}_j} \bar{\eta}_i \bar{\eta}_j + \dots \\ &\equiv \mathcal{S}_E^{\text{cl}} + \frac{\hbar}{2} \begin{pmatrix} \bar{z}_i & z_i \end{pmatrix} \begin{pmatrix} A_{ij} & B_{ij} \\ C_{ij} & A_{ij}^\dagger \end{pmatrix} \begin{pmatrix} z_j \\ \bar{z}_j \end{pmatrix} + \dots . \end{aligned} \quad (15.31)$$

For general  $H$ , we obtain

$$\begin{aligned} A_{ij} &= \delta_{ij} - \delta_{i,j+1} + \frac{\epsilon}{\hbar} \frac{\partial^2 H(\bar{z}_i|z_j)}{\partial \bar{z}_i \partial z_j} \delta_{i,j+1} \\ B_{ij} &= \frac{\epsilon}{\hbar} \frac{\partial^2 H(\bar{z}_i|z_{i-1})}{\partial \bar{z}_i^2} \delta_{i,j} \\ C_{ij} &= \frac{\epsilon}{\hbar} \frac{\partial^2 H(\bar{z}_{i+1}|z_i)}{\partial z_i^2} \delta_{i,j} \quad . \end{aligned} \quad (15.32)$$

with  $i$  and  $j$  running from 1 to  $N - 1$ . The contribution of the fluctuation determinant to the matrix element is then

$$\int \prod_{j=1}^{N-1} \frac{d^2 \eta_j}{2\pi i} \exp \left\{ -\frac{1}{2} (\text{Re } \eta_k \quad \text{Im } \eta_k) \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \begin{pmatrix} A_{kl} & B_{kl} \\ C_{kl} & A_{lk} \end{pmatrix} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \begin{pmatrix} \text{Re } \eta_l \\ \text{Im } \eta_l \end{pmatrix} \right\} = \det^{-1/2} \begin{pmatrix} A & B \\ C & A^t \end{pmatrix} \quad . \quad (15.33)$$

In the case of the harmonic oscillator discussed above, we have  $B_{ij} = C_{ij} = 0$ , and since  $A_{ij}$  has no elements above its diagonal and  $A_{ii} = 1$  for all  $i$ , we simply have that the determinant contribution is unity.

## 15.2 Coherent States for Spin

For the pros: A. Perelomov, *Generalized Coherent States and their Applications* (Springer-Verlag, NY, 1986).

A spin-coherent state  $|\hat{\Omega}\rangle$  is simply a rotation of the 'highest weight' state  $|m = +S\rangle$ , such that the spin is maximally polarized along  $\hat{\Omega}$ , *i.e.*

$$\hat{\Omega} \cdot \mathbf{S} |\hat{\Omega}\rangle = +S |\hat{\Omega}\rangle \quad . \quad (15.34)$$

Note that  $|m = +S\rangle$  is itself a coherent state with  $\hat{\Omega} = \hat{z}$ . We can effect this rotation by means of an element  $\mathcal{R}$  of the group  $\text{SU}(2)$ :

$$\begin{aligned} \mathcal{R} &\equiv \exp(i\psi S^z) \exp(i\theta S^y) \exp(i\phi S^z) \\ |\hat{\Omega}\rangle &= \mathcal{R}^\dagger |\hat{z}\rangle \quad . \end{aligned} \quad (15.35)$$

To define and manipulate the spin coherent states, it is useful to introduce the Schwinger representation of quantum spin. You are probably already familiar with the Holstein-Primakoff transformation,

$$S^+ = \hbar^\dagger (2S - \hbar^\dagger \hbar)^{1/2} \quad , \quad S^- = (2S - \hbar^\dagger \hbar)^{1/2} \hbar \quad , \quad S^z = \hbar^\dagger \hbar - S \quad , \quad (15.36)$$

with  $0 \leq h^\dagger h \leq 2S$ . by which a quantum spin can be represented by a single boson. Note that the eigenvalues of the boson number operator  $n_h = h^\dagger h$  range over the nonnegative integers. There are thus an infinite number of allowed states, but only a finite number  $(2S+1)$  of states in the Hilbert space for spin. But the factor  $\sqrt{2S - h^\dagger h}$  in  $S^+$  annihilates the state of maximal polarization,  $|m = +S\rangle$ , and thus for any Hamiltonian which can be written in terms of the spin algebra operators, the infinite-dimensional boson Hilbert space is effectively divided into two parts. The ‘physical’ states all have  $0 \leq n_h \leq 2S$ , and there are no matrix elements connecting this subspace to the ‘unphysical’ one where  $n_h > 2S$ .

The square roots are unwieldy, however, and in practice one expands them in powers of  $(n_h/2S)$ , viz.

$$(2S - h^\dagger h)^{1/2} = \sqrt{2S} \cdot \left\{ 1 - \frac{1}{2} \left( \frac{h^\dagger h}{2S} \right) + \frac{1}{8} \left( \frac{h^\dagger h}{2S} \right)^2 + \dots \right\} . \quad (15.37)$$

This expansion forms the basis of spin wave theory. Hence, within spin wave theory, unphysical states are allowed. For example, an interaction like  $S_i^+ S_j^-$  between spins on sites  $i$  and  $j$  takes the form  $2S h_i^\dagger h_j$  within the spin wave expansion. But such a term knows nothing of the border lying at  $n_h = 2S$  separating physical from unphysical states.

In the Schwinger representation, two bosons are used, and the constraint is a holonomic one (*i.e.* one which can be written as an equality):

$$S^+ = a^\dagger b \quad , \quad S^- = a b^\dagger \quad , \quad S^z = \frac{1}{2}(a^\dagger a - b^\dagger b) \quad , \quad (15.38)$$

and subject to the constraint  $a^\dagger a + b^\dagger b = 2S$ . The constraint simply says  $n_a + n_b = 2S$ , *i.e.* there are a total of  $2S$  bosons present. Note that the operators  $S^\pm$  change the number of  $a$  and  $b$  bosons, but preserve the total  $n_a + n_b$ , hence they *commute with the constraint*.

*Exercise: Verify that  $[S^+, S^-] = 2S^z$  and  $[S^z, S^\pm] = \pm S^\pm$  for both the Holstein-Primakoff and Schwinger representations.*

A shorthand way of rendering the spin operators in the Schwinger representation is

$$\mathbf{S} = \frac{1}{2} (a^\dagger \quad b^\dagger) \boldsymbol{\sigma} \begin{pmatrix} a \\ b \end{pmatrix} . \quad (15.39)$$

We now investigate the action of the  $SU(2)$  rotation  $\mathcal{R}$  on the Schwinger bosons. We wish to evaluate the expression

$$\mathcal{R}^\dagger \begin{pmatrix} a \\ b \end{pmatrix} \mathcal{R} = e^{-i\phi S^z} e^{-i\theta S^y} e^{-i\psi S^z} \begin{pmatrix} a \\ b \end{pmatrix} e^{i\psi S^z} e^{i\theta S^y} e^{i\phi S^z} . \quad (15.40)$$

Let’s work this out:

- Rotation about the  $\hat{z}$ -axis:

$$e^{-i\psi S^z} \begin{pmatrix} a \\ b \end{pmatrix} e^{i\psi S^z} = e^{-i\frac{\psi}{2} a^\dagger a} e^{i\frac{\psi}{2} b^\dagger b} \begin{pmatrix} a \\ b \end{pmatrix} e^{-i\frac{\psi}{2} b^\dagger b} e^{i\frac{\psi}{2} a^\dagger a} = \begin{pmatrix} e^{+i\frac{\psi}{2}} a \\ e^{-i\frac{\psi}{2}} b \end{pmatrix} . \quad (15.41)$$

- Rotation about the  $\hat{y}$  axis:

$$e^{-i\theta S^y} \begin{pmatrix} a \\ b \end{pmatrix} e^{i\theta S^y} = e^{\frac{\theta}{2}(ab^\dagger - a^\dagger b)} \begin{pmatrix} a \\ b \end{pmatrix} e^{-\frac{\theta}{2}(ab^\dagger - a^\dagger b)} = \begin{pmatrix} \cos(\theta/2) a + \sin(\theta/2) b \\ -\sin(\theta/2) a + \cos(\theta/2) b \end{pmatrix} . \quad (15.42)$$

We are also licensed to make an additional rotation  $\mathcal{U} = \exp(i\xi S)$ , where  $S = \frac{1}{2}(a^\dagger a + b^\dagger b)$ . The final result of the combined transformation  $\mathcal{R}\mathcal{U}$  is

$$\begin{pmatrix} \tilde{a} \\ \tilde{b} \end{pmatrix} \equiv \mathcal{U}^\dagger \mathcal{R}^\dagger \begin{pmatrix} a \\ b \end{pmatrix} \mathcal{R}\mathcal{U} = e^{i\xi/2} \begin{pmatrix} \bar{u} & v \\ -\bar{v} & u \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \quad (15.43)$$

where  $u$  and  $v$  are spinor coordinates,

$$\begin{aligned} u &= e^{-i\psi/2} e^{-i\phi/2} \cos\left(\frac{1}{2}\theta\right) \\ v &= e^{-i\psi/2} e^{+i\phi/2} \sin\left(\frac{1}{2}\theta\right) . \end{aligned} \quad (15.44)$$

The phase  $\xi$  is unphysical, and without loss of generality we are free to define  $\xi \equiv -(\phi + \psi)$ , in which case

$$\begin{pmatrix} \tilde{a} \\ \tilde{b} \end{pmatrix} = \begin{pmatrix} \cos(\frac{1}{2}\theta) & \sin(\frac{1}{2}\theta) e^{i\psi} \\ -\sin(\frac{1}{2}\theta) e^{i\phi} & \cos(\frac{1}{2}\theta) e^{-i(\phi+\psi)} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} . \quad (15.45)$$

Now that we know how the Schwinger bosons themselves transform under  $SU(2)$ , we investigate the transformation properties of the spin operators  $S^\alpha$ , which are bilinear in the Schwinger bosons. We find

$$\begin{aligned} \mathcal{R}^\dagger S^z \mathcal{R} &= \begin{pmatrix} a^\dagger & b^\dagger \end{pmatrix} \begin{pmatrix} u & -\bar{v} \\ v & \bar{u} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \bar{u} & \bar{v} \\ -v & u \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} a^\dagger & b^\dagger \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \\ &= \sin\theta \cos\phi S^x + \sin\theta \sin\phi S^y + \cos\theta S^z , \end{aligned}$$

hence  $\mathcal{R}^\dagger S^z \mathcal{R} = \hat{\Omega} \cdot \mathbf{S}$ , and

$$S | \hat{\Omega} \rangle = \mathcal{R}^\dagger S^z | \hat{z} \rangle = (\mathcal{R}^\dagger S^z \mathcal{R}) \mathcal{R}^\dagger | \hat{z} \rangle = \hat{\Omega} \cdot \mathbf{S} | \hat{\Omega} \rangle . \quad (15.46)$$

Explicitly, then,

$$| \hat{\Omega} \rangle = [(2S)!]^{-1/2} (ua^\dagger + vb^\dagger)^{2S} | 0 \rangle = \sum_{k=0}^{2S} \binom{2S}{k}^{1/2} u^k v^{2S-k} | k - S \rangle . \quad (15.47)$$

*Example:*  $S = \frac{1}{2}, \theta = \frac{1}{2}\pi, \phi = \frac{1}{2}\pi$  gives  $| \hat{\Omega} \rangle = \frac{1}{\sqrt{2}} | \uparrow \rangle + \frac{i}{\sqrt{2}} | \downarrow \rangle = | \hat{y} \rangle$ .

A useful property of the coherent states: if

$$|\psi\rangle = f(a^\dagger, b^\dagger)|0\rangle \equiv \sum_{k=0}^{2S} f_k (a^\dagger)^k (b^\dagger)^{2S-k} |0\rangle \quad , \quad (15.48)$$

then

$$\langle \hat{\Omega} | \psi \rangle = \sqrt{(2S)!} f(\bar{u}, \bar{v}) \quad , \quad (15.49)$$

*i.e.* replace  $a^\dagger \rightarrow \bar{u}$  and  $b^\dagger \rightarrow \bar{v}$  as arguments of  $f$ . The overlap of the coherent states is

$$\begin{aligned} \langle \hat{\Omega} | \hat{\Omega}' \rangle &= (\bar{u}u' + \bar{v}v')^{2S} \\ &= \left[ \frac{1}{2} (1 + \hat{\Omega} \cdot \hat{\Omega}') \right]^S e^{iS\gamma(\hat{\Omega}, \hat{\Omega}')} \end{aligned} \quad (15.50)$$

where

$$\begin{aligned} \gamma(\hat{\Omega}, \hat{\Omega}') &\equiv 2 \arg(\bar{u}u' + \bar{v}v') \\ &= 2 \tan^{-1} \left[ \frac{\sin \frac{1}{2}\theta \sin \frac{1}{2}\theta' \sin(\phi' - \phi)}{\cos \frac{1}{2}\theta \cos \frac{1}{2}\theta' + \sin \frac{1}{2}\theta \sin \frac{1}{2}\theta' \cos(\phi' - \phi)} \right] \end{aligned} \quad (15.51)$$

Perhaps the most important result, for our purposes, is the resolution of the identity:

$$1 = \frac{2S+1}{4\pi} \int d\Omega |\hat{\Omega}\rangle \langle \hat{\Omega}| \quad . \quad (15.52)$$

As with the case of coherent states for the harmonic oscillator, the spin coherent states permit a simple resolution of the identity despite their nonorthogonality.

The last step, before we tackle the derivation of the spin path integral, is to compute matrix elements in the coherent state basis. We assume that the Hamiltonian commutes with the constraint, *i.e.* it preserves total spin. The most general such Hamiltonian may be written

$$H = \sum_{m,n,j} C_{mnj} (a^\dagger)^m (b^\dagger)^n (a)^{m+j} (b)^{n-j} \quad , \quad (15.53)$$

and its matrix elements may be evaluated using

$$\langle \hat{\Omega}_1 | \overbrace{(a^\dagger)^m (b^\dagger)^n (a)^{m+j} (b)^{n-j}}^{\text{preserves total S}} | \hat{\Omega}_2 \rangle = \frac{(2S)!}{(2S-m-n)!} (\bar{u}_1 u_2 + \bar{v}_1 v_2)^{2S-m-n} \bar{u}_1^m \bar{v}_1^n u_2^{m+j} v_2^{n-j} \quad . \quad (15.54)$$

Note that the above operator product must be *normal-ordered*, with annihilation operators  $a, b$  appearing to the right of creation operators  $a^\dagger, b^\dagger$ .

*Exercise: Verify eqn. 15.54 by finding the  $\mathcal{O}(\bar{z}_1^{2S} z_2^{2S})$  term of the matrix element in the (unnormalized) generalized coherent state*

$$|z, \hat{\Omega}\rangle \equiv e^{zua^\dagger} e^{zvb^\dagger} |0\rangle \quad , \quad (15.55)$$

where  $z$  is a complex number. Show that  $a|z, \hat{\Omega}\rangle = zu|z, \hat{\Omega}\rangle$ ,  $b|z, \hat{\Omega}\rangle = zv|z, \hat{\Omega}\rangle$ , and

$$\langle z, \hat{\Omega} | z', \hat{\Omega}' \rangle = \exp[\bar{z}z'(\bar{u}u' + \bar{v}v')] \quad . \quad (15.56)$$

Use these results to verify eqn. 15.54.

As with the case of the coherent state path integral for the Heisenberg-Weyl group, only diagonal matrix elements are needed. In this case the expression eqn. 15.54 simplifies to

$$\langle \hat{\Omega} | (a^\dagger)^m (b^\dagger)^n (a)^{m+j} (b)^{n-j} | \hat{\Omega} \rangle = \frac{(2S)!}{(2S - m - n)!} \bar{u}^m \bar{v}^n u^{m+j} v^{n-j} \quad . \quad (15.57)$$

Two examples of matrix element computation:

- $\mathcal{O} = S^+ = a^\dagger b$ . Here,  $(m, n, j) = (1, 0, -1)$ , so

$$\langle \hat{\Omega} | a^\dagger b | \hat{\Omega} \rangle = 2S \bar{u}v = S \sin \theta e^{i\phi} \quad . \quad (15.58)$$

- $\mathcal{O} = (S_x)^2$ . First we normal order:

$$\begin{aligned} S_x^2 &= \left( \frac{a^\dagger b + ab^\dagger}{2} \right)^2 \\ &= \frac{1}{4} \left( a^\dagger b a^\dagger b + a b^\dagger a b^\dagger + a^\dagger b b^\dagger a + a b^\dagger a^\dagger b \right) \\ &= \frac{1}{4} \left( \overbrace{a^\dagger a^\dagger b b}^{(2,0,-2)} + \overbrace{b^\dagger b^\dagger a a}^{(0,2,2)} + 2 \overbrace{a^\dagger b^\dagger a b}^{(1,1,0)} + \overbrace{a^\dagger a}^{(1,0,0)} + \overbrace{b^\dagger b}^{(0,1,0)} \right) \quad , \end{aligned} \quad (15.59)$$

which, following the rules in Eqn. 15.57, yields

$$\begin{aligned} \langle \hat{\Omega} | S_x^2 | \hat{\Omega} \rangle &= \frac{1}{4}(2S)(2S-1)(\bar{u}^2 v^2 + \bar{v}^2 u^2 + 2\bar{u}\bar{v}uv) + \frac{1}{4}(2S)(\bar{u}u + \bar{v}v) \\ &= S(S - \frac{1}{2})(\sin \theta \cos \phi)^2 + \frac{1}{2}S \quad . \end{aligned} \quad (15.60)$$

*Exercise: Prove that*

$$\langle \hat{\Omega} | S^\alpha S^\beta | \hat{\Omega} \rangle = S(S - \frac{1}{2}) \Omega^\alpha \Omega^\beta + \frac{1}{2}S \delta_{\alpha\beta} + \frac{i}{2}S \epsilon_{\alpha\beta\gamma} \Omega^\gamma \quad . \quad (15.61)$$

### 15.2.1 Coherent state wavefunctions

Consider a state

$$|\Psi\rangle = \frac{1}{\sqrt{2S!}} \Psi(a^\dagger, b^\dagger) |0\rangle \quad , \quad (15.62)$$

where  $\Psi(a^\dagger, b^\dagger)$  is homogeneous of degree  $2S$ . Then

$$\langle \hat{\Omega} | \Psi \rangle = \Psi(\bar{u}, \bar{v}) \quad , \quad (15.63)$$

where  $\Psi(\bar{u}, \bar{v})$  is obtained from  $\Psi(a^\dagger, b^\dagger)$  simply by substituting  $a^\dagger \rightarrow \bar{u}$  and  $b^\dagger \rightarrow \bar{v}$ .

Now suppose we wish to calculate the matrix element of some operator  $\hat{A}$  between states  $|\Psi\rangle$  and  $|\Phi\rangle$ . We assume that  $\hat{A}$  preserves total spin, in which case it may be written

$$\begin{aligned} \hat{A} &= \sum_{k,l,j} A_{klj} \hat{T}_{klj} \\ \hat{T}_{klj} &= (a)^\dagger{}^k (b)^\dagger{}^l (a^\dagger)^{k+j} (b^\dagger)^{l-j} \quad . \end{aligned} \quad (15.64)$$

Note here that we have written  $\hat{A}$  in normal-ordered form, but this time with the creation operators appearing to the *right*. One then has

$$\langle \Psi | \hat{A} | \Phi \rangle = \frac{2S+1}{4\pi} \int d\Omega \langle \Psi | \hat{\Omega} \rangle \langle \hat{\Omega} | \hat{A} | \Phi \rangle \quad . \quad (15.65)$$

It can further be shown that

$$\langle \hat{\Omega} | \hat{T}_{klj} | \Phi \rangle = \left( \frac{\partial}{\partial \bar{u}} \right)^k \left( \frac{\partial}{\partial \bar{v}} \right)^l \bar{u}^{k+j} \bar{v}^{l-j} \Phi(\bar{u}, \bar{v}) \quad (15.66)$$

and that

$$\langle \Psi | \hat{T}_{klj} | \Phi \rangle = \frac{(2S+k+l+1)!}{(2S)!} \cdot \int \frac{d\Omega}{4\pi} \Psi^*(u, v) u^k v^l \bar{u}^{k+j} \bar{v}^{l-j} \Phi(\bar{u}, \bar{v}) \quad . \quad (15.67)$$

### 15.2.2 Valence bond states

The operator  $\mathcal{A}_{ij}^\dagger \equiv a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger$  creates a singlet ‘valence bond’ between sites  $i$  and  $j$ .

*Exercise: Show that  $\mathcal{A}_{ij}^\dagger$  transforms as an  $SU(2)$  singlet, i.e.  $\mathcal{R}^\dagger \mathcal{A}_{ij}^\dagger \mathcal{R} = \mathcal{A}_{ij}^\dagger$ .*

Now consider the valence bond solid (VBS) state

$$|\Psi(\mathcal{L}, m)\rangle \equiv \prod_{\langle ij \rangle \in \mathcal{L}} (a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger)^m |0\rangle \quad , \quad (15.68)$$

where  $|0\rangle$  is the Schwinger boson vacuum. Here, the product is over all links  $\langle ij \rangle$  of some regular lattice  $\mathcal{L}$ . The state  $|\Psi(\mathcal{L}, m)\rangle$  possesses the following properties:

- $|\Psi(\mathcal{L}, m)\rangle$  is a singlet, i.e. it has total spin zero.



- For every site  $i$ , we have  $(a_i^\dagger a_i + b_i^\dagger b_i) |\Psi(\mathcal{L}, m)\rangle = mz |\Psi(\mathcal{L}, m)\rangle$ , where  $z$  is the coordination number of  $\mathcal{L}$ . I.e. there is a quantum spin  $S = \frac{1}{2}mz$  at every site.
- The maximum eigenvalue of the total link spin  $\mathbf{J}_{ij} \equiv \mathbf{S}_i + \mathbf{S}_j$  is  $J_{ij}^{\max} = 2S - m$ . This is significant because with two spin- $S$  objects the total spin will in general range from 0 to  $2S$ . What is special about the VBS states is that they have zero weight in the sector  $J_{ij} > 2S - m$  for every link.

Consequently,  $|\Psi(\mathcal{L}, m)\rangle$  is annihilated by any link spin projection operator  $\mathcal{P}_S^J(ij)$ , so long as  $J > 2S - m$ . The projector  $\mathcal{P}_S^J(ij)$  may be written as an order  $2S$  polynomial in  $\mathbf{S}_i \cdot \mathbf{S}_j$ , viz.

$$\mathcal{P}_S^J(ij) = \prod_{\substack{k=0 \\ (k \neq J)}}^{2S} \frac{\mathbf{S}_i \cdot \mathbf{S}_j + S(S+1) - \frac{1}{2}k(k+1)}{\frac{1}{2}J(J+1) - \frac{1}{2}k(k+1)} . \quad (15.69)$$

Therefore, if one writes a Hamiltonian of the form

$$H = \sum_{\langle ij \rangle} \sum_{J=2S-m+1}^{2S} \lambda_J \mathcal{P}_S^J(ij) \quad (15.70)$$

with each  $\lambda_J > 0$ , then  $H|\Psi(\mathcal{L}, m)\rangle = 0$  and  $|\Psi(\mathcal{L}, m)\rangle$  is an exact, zero energy ground state for  $H$ .<sup>2</sup>

The simplest example is for the  $S = 1$  linear chain, where

$$\mathcal{P}_{S=\frac{1}{2}}^{J=1}(ij) = \frac{1}{6}(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + \frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{3} . \quad (15.71)$$

We conclude that the bilinear-biquadratic  $S = 1$  chain with Hamiltonian

$$H = J \sum_n \left[ \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \frac{1}{3}(\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2 \right] \quad (15.72)$$

has as its exact ground state  $|\Psi(\mathcal{L}, m = 1)\rangle$ , where  $\mathcal{L}$  is the linear chain. The energy per site is  $-\frac{2}{3}J$ .

The states  $|\Psi(\mathcal{L}, m)\rangle$  are easily generalized to ones of broken translational or lattice point group symmetry, even while maintaining the constraint that  $zm$  link operators  $\mathcal{A}_{ij}^\dagger$  are associated with each site  $i$  (with different values of  $j$ ).<sup>3</sup>

<sup>2</sup>If every  $\lambda_J$  is nonnegative, then it is simple to prove that  $H$  itself can have no negative eigenvalues.

<sup>3</sup>Were this not the case, then some sites would have different total spin than others. It is perfectly sensible from a mathematical point of view to consider models where the total spin varies from site to site. Most (but by no means all) models of physical interest, however, have one value of  $S$  for each magnetic site.

For example, on the honeycomb lattice, where we have links oriented along  $0^\circ$ ,  $120^\circ$ , and  $240^\circ$ , we can define the state

$$|\Psi(m, m', m'')\rangle \equiv \prod_{\langle ij \rangle \in 0^\circ} (\mathcal{A}_{ij}^\dagger)^m \prod_{\langle kl \rangle \in 120^\circ} (\mathcal{A}_{kl}^\dagger)^{m'} \prod_{\langle rs \rangle \in 240^\circ} (\mathcal{A}_{rs}^\dagger)^{m''} |0\rangle . \quad (15.73)$$

This state therefore has  $S = \frac{1}{2}(m + m' + m'')$  on each site, but it breaks the point group symmetry of the underlying triangular Bravais lattice. Similarly, one can define ‘columnar’ states on the square lattice which break both translational and point group symmetry, *e.g.*

$$\begin{aligned} |\Psi_A\rangle &= \prod_{m,n} (a_{m,n}^\dagger b_{m+1,n}^\dagger - b_{m,n}^\dagger a_{m+1,n}^\dagger) |0\rangle \\ |\Psi_B\rangle &= \prod_{j,n} (a_{2j,n}^\dagger b_{2j+1,n}^\dagger - b_{2j,n}^\dagger a_{2j+1,n}^\dagger)^2 |0\rangle . \end{aligned} \quad (15.74)$$

*Exercise: Compare and contrast the states  $|\Psi_A\rangle$  and  $|\Psi_B\rangle$ .*

### 15.2.3 Derivation of spin path integral

Let us compute the real time propagator in the coherent state basis. We begin, as usual, by writing

$$\langle \hat{\Omega}_N | e^{-iHT/\hbar} | \hat{\Omega}_0 \rangle = \langle \hat{\Omega}_N | e^{-i\epsilon H/\hbar} 1 e^{-i\epsilon H/\hbar} 1 \dots 1 e^{-i\epsilon H/\hbar} | \hat{\Omega}_0 \rangle , \quad (15.75)$$

where each symbol 1 stands for an insertion of the resolution of the identity, eqn. 15.52. We next compute

$$\begin{aligned} \langle \hat{\Omega}_j | e^{-i\epsilon H/\hbar} | \hat{\Omega}_{j-1} \rangle &= \langle \hat{\Omega}_j | \hat{\Omega}_{j-1} \rangle \cdot \left\{ 1 - \frac{i\epsilon}{\hbar} \frac{\langle \hat{\Omega}_j | H | \hat{\Omega}_{j-1} \rangle}{\langle \hat{\Omega}_j | \hat{\Omega}_{j-1} \rangle} + \mathcal{O}(\epsilon^2) \right\} \\ &\simeq \langle \hat{\Omega}_j | \hat{\Omega}_{j-1} \rangle \exp \left( -i\epsilon H(\hat{\Omega}_j | \hat{\Omega}_{j-1})/\hbar \right) , \end{aligned} \quad (15.76)$$

where the Hamiltonian is replaced by its coherent state matrix element,

$$H(\hat{\Omega}_j | \hat{\Omega}_{j-1}) = \frac{\langle \hat{\Omega}_j | H | \hat{\Omega}_{j-1} \rangle}{\langle \hat{\Omega}_j | \hat{\Omega}_{j-1} \rangle} . \quad (15.77)$$

*Exercise: Show that  $H(\hat{\Omega}_j | \hat{\Omega}_{j-1}) = H(\bar{u}_j, \bar{v}_j | u_{j-1}, v_{j-1})$  is a holomorphic function of its arguments.*

We therefore have

$$\langle \hat{\Omega}_N | e^{-iHT/\hbar} | \hat{\Omega}_0 \rangle = \left( \frac{2S+1}{4\pi} \right)^{N-1} \int d\Omega_1 \dots \int d\Omega_{N-1} e^{i\mathcal{A}\{\{\hat{\Omega}_j\}\}} , \quad (15.78)$$

where  $\mathcal{A} \equiv S/\hbar$  is given by

$$\mathcal{A} = -i \sum_{j=1}^N \ln \langle \hat{\Omega}_j | \hat{\Omega}_{j-1} \rangle - \frac{\epsilon}{\hbar} \sum_{j=1}^N H(\hat{\Omega}_j | \hat{\Omega}_{j-1}) \quad . \quad (15.79)$$

Expanding in the difference between  $\hat{\Omega}_j$  and  $\hat{\Omega}_{j-1}$ , we may write

$$\begin{aligned} \ln \langle \hat{\Omega}_j | \hat{\Omega}_{j-1} \rangle &= 2S \ln \left\{ 1 - \bar{u}_j(u_j - u_{j-1}) - \bar{v}_j(v_j - v_{j-1}) \right\} \\ &= -2S \epsilon \left\{ \bar{u}_j \left( \frac{u_j - u_{j-1}}{\epsilon} \right) - \bar{v}_j \left( \frac{v_j - v_{j-1}}{\epsilon} \right) + \dots \right\} \\ &\simeq -2S \epsilon (\bar{u}_j \dot{u}_j + \bar{v}_j \dot{v}_j) + \mathcal{O}((\hat{\Omega}_j - \hat{\Omega}_{j-1})^2) \quad . \end{aligned} \quad (15.80)$$

The continuum limit is

$$\mathcal{A}[\hat{\Omega}(t)] = \int_0^T dt \left\{ 2iS(\bar{u}\dot{u} + \bar{v}\dot{v}) - \frac{1}{\hbar} H(\hat{\Omega}) \right\} \quad , \quad (15.81)$$

where  $H(\hat{\Omega}) \equiv H(\hat{\Omega} | \hat{\Omega})$ . Substituting  $u = \cos(\theta/2)$  and  $v = \sin(\theta/2) \exp(i\phi)$ , we obtain

$$\bar{u}\dot{u} + \bar{v}\dot{v} = i \sin^2(\theta/2) \dot{\phi} = \frac{i}{2}(1 - \cos \theta) \dot{\phi} = \frac{i}{2} \dot{\omega} \quad (15.82)$$

where  $d\omega = (1 - \cos \theta) d\phi$  is the differential element of solid angle. We may now, finally, write the spin path integral as

$$\langle \hat{\Omega}_f | e^{-iHT/\hbar} | \hat{\Omega}_i \rangle = \int_{\substack{w(0)=w_i \\ \bar{w}(T)=\bar{w}_f}} \mathcal{D}\hat{\Omega}(t) \exp \left\{ -i \int_0^T dt \left[ S \frac{d\omega}{dt} + \frac{1}{\hbar} H(\hat{\Omega}) \right] \right\} \cdot \langle \hat{\Omega}_f | \hat{\Omega}(T) \rangle \langle \hat{\Omega}(0) | \hat{\Omega}_i \rangle \quad (15.83)$$

where  $w \equiv v/u = \tan(\theta/2) \exp(i\phi)$  is the stereographic projection of the spinor coordinates  $(u, v)$  onto the complex plane.

The inclusion of the overlap terms inside the path integral is necessary if we are to allow for the possibility of so-called discontinuous paths. Within the semiclassical approximation,  $u(t)$  and  $v(t)$  are integrated forward from initial data  $u_i$  and  $v_i$  while  $\bar{u}(t)$  and  $\bar{v}(t)$  are integrated backward from final data  $\bar{u}_f$  and  $\bar{v}_f$ .<sup>4</sup> We encountered an analogous situation with the coherent state path integral for the Heisenberg-Weyl group, where  $z(t)$  was integrated forward from initial data  $z_i$  and  $\bar{z}(t)$  integrated backward from final data  $\bar{z}_f$ . In fact, these paths are perfectly continuous; there simply is no reason why  $z(T)$  should have any resemblance to  $z_f$ , or  $\bar{z}(0)$  to  $\bar{z}_i$ , since the equations of motion know nothing about either  $z_f$  or  $\bar{z}_i$ .

<sup>4</sup>The equations of motion may also be written in terms of the stereographic coordinate  $w = v/u$ , in which case  $w(t)$  is integrated forward from initial data  $w_i$  and  $\bar{w}(t)$  is integrated backward from final data  $\bar{w}_f$ .

The thermal, or imaginary time, propagator in the coherent state representation is

$$\langle \hat{\Omega}_f | e^{-\beta H} | \hat{\Omega}_i \rangle = \int_{\substack{w(0)=w_i \\ \bar{w}(T)=\bar{w}_f}} \mathcal{D}\hat{\Omega}(\tau) \exp \left\{ - \int_0^{\hbar\beta} d\tau \left[ iS \frac{d\omega}{d\tau} + \frac{1}{\hbar} H(\hat{\Omega}) \right] \right\} \cdot \langle \hat{\Omega}_f | \hat{\Omega}(\hbar\beta) \rangle \langle \hat{\Omega}(0) | \hat{\Omega}_i \rangle \quad . \quad (15.84)$$

### 15.2.4 Gauge field and geometric phase

The solid angle functional  $\omega[\hat{\Omega}(t)]$  may be written

$$\omega[\hat{\Omega}(t)] = \int_0^T dt \mathbf{A}(\hat{\Omega}) \cdot \frac{d\hat{\Omega}}{dt} \quad (15.85)$$

for any  $\mathbf{A}(\hat{\Omega})$  which satisfies  $\nabla \times \mathbf{A} = \hat{\Omega}$ , *i.e.*

$$\Omega^a = \epsilon_{abc} \frac{\partial}{\partial \Omega^b} A^c(\hat{\Omega}) \quad (15.86)$$

(To see this, use Stokes' theorem.) We now derive a useful result:

$$\begin{aligned} \delta\omega[\hat{\Omega}(t)] &= \int dt \left\{ \frac{\partial A^b}{\partial \Omega^a} \frac{d\Omega^b}{dt} \delta\Omega^a + A^a \frac{d}{dt} \delta\Omega^a \right\} \\ &= \int dt \left( \frac{\partial A^b}{\partial \Omega^a} - \frac{\partial A^a}{\partial \Omega^b} \right) \frac{d\Omega^b}{dt} \delta\Omega^a \\ &= \int dt \delta\Omega^a \epsilon_{abc} \dot{\Omega}^b \Omega^c = \int dt \delta\hat{\Omega} \cdot \frac{\partial \hat{\Omega}}{\partial t} \times \hat{\Omega} \quad , \end{aligned} \quad (15.87)$$

and hence the functional derivative is

$$\frac{\delta\omega[\hat{\Omega}]}{\delta\hat{\Omega}(t)} = \frac{\partial \hat{\Omega}}{\partial t} \times \hat{\Omega} \quad . \quad (15.88)$$

### 15.2.5 Semiclassical dynamics

We begin with the action functional,

$$\tilde{\mathcal{A}}[\hat{\Omega}(t), \lambda(t)] \equiv \mathcal{A}[\hat{\Omega}(t)] + \int_0^T dt \lambda(t) (\hat{\Omega}^2(t) - 1) \quad . \quad (15.89)$$

Here,  $\lambda(t)$  is a Lagrange multiplier field which enforces the constraint  $\hat{\Omega}(t) \cdot \hat{\Omega}(t) = 1$  at all times. We next vary with respect to  $\hat{\Omega}(t)$  and  $\lambda(t)$ :

$$\begin{aligned} \frac{\delta \tilde{\mathcal{A}}}{\delta \hat{\Omega}(t)} &= -S \frac{\partial \hat{\Omega}}{\partial t} \times \hat{\Omega} - \frac{1}{\hbar} \frac{\partial H}{\partial \hat{\Omega}} + 2\lambda \hat{\Omega} \\ \frac{\delta \tilde{\mathcal{A}}}{\delta \lambda(t)} &= \hat{\Omega}^2(t) - 1 \quad . \end{aligned} \quad (15.90)$$

Setting these variations to zero, we solve for  $\lambda(t)$  by taking the dot product of the first equation with  $\hat{\Omega}(t)$  and then substituting  $\hat{\Omega}^2(t) = 1$ . In this manner, we find

$$\lambda = \frac{1}{2\hbar} \frac{\partial H}{\partial \hat{\Omega}} \cdot \hat{\Omega} \quad , \quad (15.91)$$

The effect of this is to render all terms on the RHS of eqn. 15.90 orthogonal to  $\hat{\Omega}$ , thereby effectively projecting  $\partial H / \partial \hat{\Omega}$  onto this orthogonal subspace. It is then easy to obtain the equations of motion

$$\hbar S \frac{\partial \hat{\Omega}}{\partial t} = \frac{\partial H}{\partial \hat{\Omega}} \times \hat{\Omega} \quad . \quad (15.92)$$

If we write the equations of motion in terms of the spinor coordinates  $\{u, v, \bar{u}, \bar{v}\}$  themselves, it is important to recognize that they must satisfy the constraint  $u\bar{u} + v\bar{v} = 1$ . A Lagrange multiplier field  $\lambda$  is invoked to impose this constraint at every value of the time  $t$ . This results in the equations of motion

$$2i\hbar S \dot{u} = \frac{\partial H}{\partial \bar{u}} + \lambda u \quad \quad \quad 2i\hbar S \dot{v} = \frac{\partial H}{\partial \bar{v}} + \lambda v \quad (15.93)$$

$$-2i\hbar S \dot{\bar{u}} = \frac{\partial H}{\partial u} + \lambda \bar{u} \quad \quad \quad -2i\hbar S \dot{\bar{v}} = \frac{\partial H}{\partial v} + \lambda \bar{v} \quad . \quad (15.94)$$

Varying the action with respect to the Lagrange multiplier field of course yields the constraint equation. We are then left with five equations in the five unknowns  $\{u, v, \bar{u}, \bar{v}, \lambda\}$ , along with the four boundary conditions,

$$u(0) = u_i \quad , \quad \bar{u}(T) = \bar{u}_f \quad , \quad v(0) = v_i \quad , \quad \bar{v}(T) = \bar{v}_f \quad . \quad (15.95)$$

Implementing the constraint, one obtains an expression for  $\lambda$ ,

$$\lambda = 2iS(\bar{u}\dot{u} + \bar{v}\dot{v}) - \bar{u} \frac{\partial H}{\partial \bar{u}} - \bar{v} \frac{\partial H}{\partial \bar{v}} \quad (15.96)$$

$$= -2iS(u\dot{\bar{u}} + v\dot{\bar{v}}) - u \frac{\partial H}{\partial u} - v \frac{\partial H}{\partial v} \quad . \quad (15.97)$$

Note that for real  $\theta$  and  $\phi$  that eqns. 15.93 and eqn. 15.94 are related by complex conjugation.

## 15.3 Other Useful Representations of the Spin Path Integral

### 15.3.1 Stereographic representation

In the stereographic representation, we write

$$w \equiv \frac{v}{u} = \tan(\theta/2) e^{i\phi} \quad . \quad (15.98)$$

One then finds

$$\frac{\bar{w}\dot{w}}{1+\bar{w}w} = \bar{u}\dot{u} + \bar{v}\dot{v} - \frac{d}{dt} \ln u \quad . \quad (15.99)$$

From the differential

$$dw = \frac{1}{2} \sec^2(\theta/2) e^{i\phi} d\theta + i \tan(\theta/2) e^{i\phi} d\phi \quad , \quad (15.100)$$

we obtain

$$\frac{dw \wedge d\bar{w}}{(1+\bar{w}w)^2} = \frac{1}{2i} \sin \theta d\theta \wedge d\phi \quad . \quad (15.101)$$

The Hamiltonian matrix elements may be recast in terms of  $w$  and  $\bar{w}$ . For example,

$$\begin{aligned} S^+ = a^\dagger b &\longrightarrow 2S \bar{w}v = \frac{2S w}{1+\bar{w}w} \\ S^z = \frac{1}{2}(a^\dagger a - b^\dagger b) &\longrightarrow S(\bar{u}u - \bar{v}v) = S \frac{1-\bar{w}w}{1+\bar{w}w} \quad . \end{aligned} \quad (15.102)$$

Thus, the real and imaginary time path integrals are given by

$$\langle \hat{\Omega}_f | e^{-iHT/\hbar} | \hat{\Omega}_i \rangle = \int \mathcal{D}[\bar{w}(t), w(t)] \exp \left\{ -i \int_0^T dt \left[ -iS \frac{\bar{w}\dot{w} - \dot{\bar{w}}w}{1+\bar{w}w} + \frac{1}{\hbar} H(\bar{w}, w) \right] \right\} \quad (15.103)$$

and

$$\langle \hat{\Omega}_f | e^{-HT/\hbar} | \hat{\Omega}_i \rangle = \int \mathcal{D}[\bar{w}(t), w(t)] \exp \left\{ - \int_0^T dt \left[ S \frac{\bar{w}\dot{w} - \dot{\bar{w}}w}{1+\bar{w}w} + \frac{1}{\hbar} H(\bar{w}, w) \right] \right\} \quad , \quad (15.104)$$

respectively. In these above expressions, the metric  $\mathcal{D}[\bar{w}, w]$  includes the  $(1+\bar{w}w)^{-2}$  factor at each time step, and the Hamiltonian  $H(\bar{w}, w)$  is the coherent state diagonal matrix element expressed in terms of the stereographic coordinate  $w$  and its conjugate  $\bar{w}$ . These expressions are incomplete, however, in that we've omitted the boundary overlap factors at  $t=0$  and  $t=T$ .

*Exercise: Complete the expression in eqns. 15.103 and 15.104, adding the boundary terms.*

### 15.3.2 Recovery of spin wave theory

To recover spin wave theory and the Holstein-Primakoff transformation, define  $z \equiv u\bar{v}/|v| = \cos(\theta/2) \exp(-i\phi)$ . Then  $|z|^2 = |u|^2$  and

$$dz = -\frac{1}{2} \sin(\theta/2) e^{-i\phi} d\theta - i \cos(\theta/2) e^{-i\phi} d\phi \quad . \quad (15.105)$$

We then obtain

$$dz \wedge d\bar{z} = \frac{1}{2i} \sin \theta d\theta \wedge d\phi \quad . \quad (15.106)$$

The geometrical phase, which is responsible for the  $\omega[\hat{\Omega}(t)]$  term in the action functional, is obtained using

$$\bar{z}\dot{z} = \frac{i}{2} (1 - \cos \theta) d\phi - i d\phi + d \cos^2(\theta/2) \quad (15.107)$$

which, after dropping the total time derivatives, yields  $(i/2) d\omega$ . As for the Hamiltonian, we have

$$\begin{aligned} S^+ = a^\dagger b &\longrightarrow 2S \bar{u}v = 2S \bar{z} \sqrt{1 - \bar{z}z} \\ S^z = \frac{1}{2}(a^\dagger a - b^\dagger b) &\longrightarrow S(\bar{u}u - \bar{v}v) = 2S(\bar{z}z - \frac{1}{2}) \quad . \end{aligned} \quad (15.108)$$

This is equivalent to Holstein-Primakoff, with  $h \equiv \sqrt{2S} z$  as the HP boson. We therefore obtain

$$\langle \hat{\Omega}_f | e^{-iHT/\hbar} | \hat{\Omega}_i \rangle = \int \mathcal{D}[\bar{h}(t), h(t)] \exp \left\{ -i \int_0^T dt \left[ \bar{h}\dot{h} + \frac{1}{\hbar} H(\bar{h}, h) \right] \right\} \quad , \quad (15.109)$$

where the functional integration is over a disk of area  $2\pi S$  for each time  $t$ .

## 15.4 Quantum Tunneling of Spin

### 15.4.1 Model Hamiltonian

The theory of quantum spin tunneling has been developed largely by E. Chudnovsky, A. Garg, D. Loss, and others. Consider the following model Hamiltonian,

$$H = K_1 S_z^2 + K_2 S_y^2 - \gamma H S_z \quad , \quad (15.110)$$

where  $K_1 > K_2 > 0$ . This describes a spin- $S$  particle with an easy axis along  $\hat{x}$  and a hard axis along  $\hat{z}$ . To treat this problem by the coherent state path integral, we need to compute the diagonal matrix element of  $H$  in the coherent state basis. One finds,

$$E(\theta, \phi) = \langle \hat{\Omega} | H | \hat{\Omega} \rangle = k_1 \cos^2 \theta + k_2 \sin^2(\theta) \sin^2(\phi) - h \cos(\theta) \quad , \quad (15.111)$$

where  $k_i = S(S - \frac{1}{2})K_i$  ( $i = 1, 2$ ),  $h = \gamma SH$ , and where we have dropped an unimportant constant. In weak fields  $h$ , the energy function  $E(\theta, \phi)$  has the following features:

- $E(\theta, \phi)$  has two degenerate minima with  $\theta_0 = \cos^{-1}(h/2k_1)$  at  $\phi = 0$  and at  $\phi = \pi$ . The minimum energy is  $E_0^{\text{cl}} = -h^2/4k_1$ .
- There is a global maximum with  $E_{\text{max}} = k_1 + h$  located (assuming  $h > 0$ ) at the South Pole ( $\theta = \pi$ ), and a local maximum with  $E'_{\text{max}} = k_1 - h$  located at the North Pole ( $\theta = 0$ ).
- There are two saddle points, located at  $\theta_x = \cos^{-1}(h/2(k_1 - k_2))$ , with  $\phi = \pm\frac{1}{2}\pi$ . The energy of the saddle points is  $E_{\text{saddle}} = k_2 - \frac{1}{4}h^2/(k_1 - k_2)$ .

We therefore expect to find two low-lying states which are linear combinations of the coherent states  $|\theta = \theta_0, \phi = 0\rangle$  and  $|\theta = \theta_0, \phi = \pi\rangle$ . Let us abbreviate these two states  $|0\rangle$  and  $|\pi\rangle$ , respectively. The eigenstates of the system should be symmetric and antisymmetric combinations of these states:  $|\pm\rangle = 2^{-1/2}\{|0\rangle \pm |\pi\rangle\}$ . The tunnel splitting  $\Delta = E_0$  may be obtained by examining the matrix elements,

$$\begin{aligned} \langle + | e^{-\beta H} | + \rangle &= \langle 0 | e^{-\beta H} | 0 \rangle + \langle 0 | e^{-\beta H} | \pi \rangle = e^{-\beta E_0} \\ \langle - | e^{-\beta H} | - \rangle &= \langle 0 | e^{-\beta H} | 0 \rangle - \langle 0 | e^{-\beta H} | \pi \rangle = e^{-\beta(E_0 + \Delta)} \end{aligned} \quad (15.112)$$

where  $E_0$  differs from  $E_0^{\text{cl}}$  due to ‘zero-point energy’, *i.e.* quantum fluctuations. In reality, there is no reason why the states  $|\pm\rangle$  should necessarily be eigenstates of  $H$ . What is important, though, is that the antisymmetric combination projects out all of the ground state. By taking the  $\beta \rightarrow \infty$  limit, the contribution from admixtures of higher-lying eigenstates to  $|\pm\rangle$  can be suppressed. What this means is that we can calculate the exact tunnel splitting by the formula,

$$\Delta = \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln \left\{ \frac{\langle 0 | e^{-\beta H} | 0 \rangle + \langle 0 | e^{-\beta H} | \pi \rangle}{\langle 0 | e^{-\beta H} | 0 \rangle - \langle 0 | e^{-\beta H} | \pi \rangle} \right\} . \quad (15.113)$$

Another way, of course, to compute the tunnel splitting is to simply numerically diagonalize the rank- $(2J + 1)$  Hamiltonian matrix. This works without fail, but it is not particularly instructive in elucidating the physics of spin tunneling. Moreover, it may be that an instanton calculation, which we shall presently describe, yields certain analytic results which are useful and in general impossible to obtain numerically.

## 15.4.2 Instantons and tunnel splittings

The essence of the instanton approach to quantum tunneling is described in a beautiful article by Sidney Coleman, entitled “The Uses of Instantons”. We write the imaginary time matrix element  $\langle P_f | \exp(-\beta H) | P_i \rangle$  between points  $P_1$  and  $P_2$  as a path integral. In our case, each  $P$  labels a spin orientation  $\hat{\mathcal{Q}}$ , and each state  $|P\rangle$  is a spin coherent state. We extremize the action, applying the method of stationary phase. This involves solving the classical equations



of motion, subject to boundary conditions which we shall not fully specify, save to say that the most naïve boundary conditions are simply  $\hat{\Omega}(0) = \hat{\Omega}_i$  and  $\hat{\Omega}(\hbar\beta) = \hat{\Omega}_f$ .<sup>5</sup>

There may be several instanton paths connecting  $P_1$  and  $P_2$ . Associated with each such instanton  $\alpha$  is a characteristic time  $\tau_\alpha$ , a classical action  $Y_\alpha + i\phi_\alpha$ , written in units of  $\hbar$  and separating real and imaginary parts, and also a ‘fluctuation determinant’ prefactor  $D_\alpha$  arising from integrating over Gaussian fluctuations about the classical instanton trajectory. If we write

$$\xi_\alpha = D_\alpha e^{i\phi_\alpha} e^{-Y_\alpha} \quad , \quad (15.114)$$

then the diagonal matrix element can be written in the ‘dilute instanton gas’ approximation as

$$\begin{aligned} \langle P_1 | e^{-\beta H} | P_1 \rangle &= \sum_{n=0}^{\infty} \sum_{\{\alpha_k, \bar{\alpha}_k\}} \int_0^{\hbar\beta} d\tau_1 \cdots \int_{\tau_{2n-1}}^{\hbar\beta} d\tau_{2n} \xi_{\alpha_1} \xi_{\bar{\alpha}_1} \cdots \xi_{\bar{\alpha}_n} \\ &= \cosh \left( \hbar\beta \left| \sum_{\alpha} \xi_{\alpha} \right| \right) \quad . \end{aligned} \quad (15.115)$$

Here we denote the return instantons from  $P_2$  to  $P_1$  with the index  $\bar{\alpha}$ . Since the return path is a time-reversed one, we have  $\xi_{\bar{\alpha}} = \overline{\xi_{\alpha}}$ , *i.e.* the return paths have opposite phase.

The off-diagonal matrix element, in which paths must begin at  $P_1$  and end at  $P_2$  requires an odd number of instanton events, and is given by

$$\begin{aligned} \langle P_2 | e^{-\beta H} | P_1 \rangle &= \sum_{n=0}^{\infty} \sum_{\{\alpha_k, \bar{\alpha}_k\}} \int_0^{\hbar\beta} d\tau_1 \cdots \int_{\tau_{2n}}^{\hbar\beta} d\tau_{2n+1} \xi_{\alpha_1} \xi_{\bar{\alpha}_1} \cdots \xi_{\bar{\alpha}_n} \xi_{\alpha_{n+1}} \\ &= \frac{\sum_{\alpha} \xi_{\alpha}}{\left| \sum_{\alpha} \xi_{\alpha} \right|} \cdot \sinh \left( \hbar\beta \left| \sum_{\alpha} \xi_{\alpha} \right| \right) \quad . \end{aligned} \quad (15.116)$$

If  $\sum_{\alpha} \xi_{\alpha}$  is real, then we can read off the tunnel splitting:

$$\Delta = 2\hbar \sum_{\alpha} D_{\alpha} e^{i\phi_{\alpha}} e^{-Y_{\alpha}} \quad . \quad (15.117)$$

### 15.4.3 Garg’s calculation (1993)

Starting from the Euclidean Lagrangian,

$$L_E = i\hbar S(1 - \cos \theta) \dot{\phi} + E(\theta, \phi) \quad , \quad (15.118)$$

<sup>5</sup>In fact, the proper boundary conditions are  $u(0) = u_i$ ,  $v(0) = v_i$ ,  $\bar{u}(\hbar\beta) = \bar{u}_f$ , and  $\bar{v}(\hbar\beta) = \bar{v}_f$ , as derived above.

one derives the Euler-Lagrange equations of motion,

$$\begin{aligned} \frac{\partial L_E}{\partial \theta} - \frac{d}{dt} \frac{\partial L_E}{\partial \dot{\theta}} = 0 &= \frac{1}{\hbar} \frac{\partial E}{\partial \theta} + iS \sin(\theta) \dot{\phi} \\ \frac{\partial L_E}{\partial \phi} - \frac{d}{dt} \frac{\partial L_E}{\partial \dot{\phi}} = 0 &= \frac{1}{\hbar} \frac{\partial E}{\partial \phi} - iS \sin(\theta) \dot{\theta} \quad . \end{aligned} \quad (15.119)$$

Note that

$$\frac{dE}{dt} = \dot{\theta} \frac{\partial E}{\partial \theta} + \dot{\phi} \frac{\partial E}{\partial \phi} = 0 \quad , \quad (15.120)$$

which says that the energy  $E(\theta, \phi)$  is conserved along the classical trajectories. One can use this result to finesse the instanton calculation and solve directly for  $\theta$  as a function of  $\phi$ . Energy conservation provides a quadratic equation in  $\cos(\theta)$ ,

$$E_0 = -\frac{h^2}{4k_1} = k_1 \cos^2(\theta) + k_2 \sin^2(\theta) \sin^2 \phi - h \cos(\theta) \quad , \quad (15.121)$$

the solution of which is written (Garg, 1993),

$$u(\phi) = \frac{u_0 + i\sqrt{\lambda} \sin \phi \sqrt{1 - u_0^2 - \lambda \sin^2 \phi}}{1 - \lambda \sin^2 \phi} \quad (15.122)$$

where  $u \equiv \cos(\theta)$ ,  $u_0 = h/2k_1 \equiv h/h_c$ , and  $\lambda = k_2/k_1$ . Note that  $u = \cos \theta$  is complex along the instanton path. Nevertheless, the path obeys the boundary condition that  $u = u_0$  at  $\phi = 0$  and  $\phi = \pi$ . The dimensionless instanton action is

$$\mathcal{A} = Y + i\phi = \beta E_0 + iS \int_0^{\pm\pi} d\phi \{1 - u(\phi)\} \quad , \quad (15.123)$$

whence

$$\phi = \text{Im } \mathcal{A} = \pm S \int_0^{\pi} d\phi \left\{ 1 - \frac{u_0}{1 - \lambda \sin^2 \phi} \right\} = \pm \pi S \left\{ 1 - \frac{u_0}{\sqrt{1 - \lambda^2}} \right\} \quad . \quad (15.124)$$

Thus, there are two instantons connecting  $(\theta, \phi) = (\theta_0, 0)$  and  $(\theta, \phi) = (\theta_0, \pi)$  which wind around the sphere in opposite directions. The tunnel splitting, according to eqn. 15.117, is

$$\Delta = 4D e^{-Y} \cos \left( \pi S \left[ 1 - \frac{h}{2\sqrt{k_1^2 - k_2^2}} \right] \right) \quad . \quad (15.125)$$

The tunnel splitting therefore vanishes at a set of dimensionless field strengths  $h_m$ , where

$$h_m = 2\sqrt{k_1^2 - k_2^2} \left\{ 1 - \frac{m + \frac{1}{2}}{S} \right\} \quad . \quad (15.126)$$

Note that for  $h = 0$  the splitting vanishes whenever  $S = m + \frac{1}{2}$ , which is to say whenever the ground state is a Kramers doublet.

In  $\text{Fe}_8$  clusters, where  $S = 10$ , this predicts ten values of  $h > 0$  where  $\Delta$  vanishes. In fact, experiments by Wernsdorfer and Sessoli see only four such vanishings. The reason for this is that the effective Hamiltonian for the experimental molecule includes a term proportional to  $J_+^4 + J_-^4$  which is not included in the Hamiltonian of eqn. 15.110. This new term allows for two additional instanton solutions. Moreover, the new solutions exhibit discontinuities in  $\hat{\Omega}(\tau)$  at the boundaries  $\tau = 0$  and  $\tau = \hbar\beta$ . This very interesting result was obtained by Keçecioglu and Garg (2002).

## 15.5 Haldane's Mapping to the Nonlinear Sigma Model

The many-spin dimensionless action is

$$\mathcal{A} = -S \sum_i \omega[\hat{\Omega}_i(t)] - \frac{1}{\hbar} \int_0^T dt H(\{\hat{\Omega}_i(t)\}) \quad , \quad (15.127)$$

where the Hamiltonian is that of a Heisenberg antiferromagnet, with diagonal coherent state matrix elements given by

$$H(\{\hat{\Omega}_i(t)\}) = \frac{1}{2} S^2 \sum_{i,j} J_{ij} \hat{\Omega}_i \cdot \hat{\Omega}_j \quad , \quad (15.128)$$

where  $J_{ij} = J(|\mathbf{R}_{ij}|)$  with  $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$  is a function of the distance between sites  $i$  and  $j$  in the lattice. The spin coherent state at site  $i$  is polarized along the direction

$$\hat{\Omega}_i = \eta_i \hat{n}_i \sqrt{1 - \left(\frac{v_0 \mathbf{L}_i}{\hbar S}\right)^2} + \frac{v_0}{\hbar S} \mathbf{L}_i \quad , \quad (15.129)$$

where  $\hat{n}_i \cdot \mathbf{L}_i = 0$ . Here,  $\hat{n}_i$  is the local Néel field, which varies slowly once the sublattice modulation  $\eta_i$  extracted from the spin field  $\hat{\Omega}_i$ ,  $\mathbf{L}_i$  describes ferromagnetic fluctuations about the local Néel order;  $v_0$  is the unit cell volume. Note that

$$\hbar S \sum_i \hat{\Omega}_i = v_0 \sum_i \mathbf{L}_i = \int d^d x \mathbf{L}(x) \quad , \quad (15.130)$$

where the RHS is obtained after taking the continuum limit.

### 15.5.1 Hamiltonian

We now expand the Heisenberg interaction  $\hat{\Omega}_i \cdot \hat{\Omega}_j$  in the slowly varying quantities  $\hat{n}_i - \hat{n}_j$  and  $L_i$ . Since  $\hat{n}_i$  is a unit vector, we may write

$$\hat{n}_i \cdot \hat{n}_j = 1 - \frac{1}{2}(\hat{n}_i - \hat{n}_j) \cdot (\hat{n}_i - \hat{n}_j) \quad . \quad (15.131)$$

We then have

$$\begin{aligned} \hat{\Omega}_i \cdot \hat{\Omega}_j &= \eta_i \eta_j \left\{ 1 - \frac{1}{2}(\hat{n}_i - \hat{n}_j) \cdot (\hat{n}_i - \hat{n}_j) \right\} \left\{ 1 - \frac{1}{2} \left( \frac{v_0}{\hbar S} \right) (\mathbf{L}_i^2 + \mathbf{L}_j^2) + \dots \right\} \\ &+ \frac{v_0}{\hbar S} \eta_i \hat{n}_i \cdot (\mathbf{L}_j - \mathbf{L}_i) + \frac{v_0}{\hbar S} \eta_j \hat{n}_j \cdot (\mathbf{L}_i - \mathbf{L}_j) \\ &+ \frac{1}{2} \left( \frac{v_0}{\hbar S} \right)^2 \left\{ \mathbf{L}_i^2 + \mathbf{L}_j^2 - (\mathbf{L}_i - \mathbf{L}_j)^2 \right\} \quad . \end{aligned} \quad (15.132)$$

Lattice differences may now be expanded in derivatives, as

$$f(\mathbf{R}_j) - f(\mathbf{R}_i) = (R_j^\mu - R_i^\mu) \frac{\partial f(\mathbf{R}_i)}{\partial R_i^\mu} + \frac{1}{2} (R_j^\mu - R_i^\mu) (R_j^\nu - R_i^\nu) \frac{\partial^2 f(\mathbf{R}_i)}{\partial R_i^\mu \partial R_i^\nu} + \dots \quad (15.133)$$

Expanding to Gaussian order in the fields  $\hat{n}$  and  $L$  and their gradients, we find

$$\begin{aligned} \hat{\Omega}_i \cdot \hat{\Omega}_j &= \eta_i \eta_j \left\{ 1 - \frac{1}{2} (R_j^\mu - R_i^\mu) (R_j^\nu - R_i^\nu) (\partial_\mu n_i^a) (\partial_\nu n_i^a) + \dots \right\} \\ &+ \frac{1}{2} \left( \frac{v_0}{\hbar S} \right)^2 \left\{ (1 - \eta_i \eta_j) (\mathbf{L}_i^2 + \mathbf{L}_j^2) - (R_j^\mu - R_i^\mu) (R_j^\nu - R_i^\nu) (\partial_\mu L_i^a) (\partial_\nu L_i^a) + \dots \right\} \\ &+ \frac{v_0}{\hbar S} \eta_i n_i^a (R_j^\mu - R_i^\mu) (\partial_\mu L_i^a) - \frac{v_0}{\hbar S} \eta_j n_j^a (R_j^\mu - R_i^\mu) (\partial_\mu L_j^a) + \dots \quad . \end{aligned} \quad (15.134)$$

Upon performing the double sum over lattice sites  $i$  and  $j$ , the terms on the last line vanish, and we are left with

$$H = H_{\hat{n}} + H_L + E_0 \quad (15.135)$$

where the classical energy  $E_0$  is given by

$$E_0 = \frac{1}{2} S^2 \sum_{i,j} J_{ij} \eta_i \eta_j \quad . \quad (15.136)$$

The Hamiltonian also contains contributions due to gradients in the Néel field,

$$H_{\hat{n}} = -\frac{S^2}{4d\mathcal{N}v_0} \sum_{i,j} J_{ij} \eta_i \eta_j |\mathbf{R}_i - \mathbf{R}_j|^2 \cdot \int d^d x (\partial_\mu n^a)^2 \quad (15.137)$$

where  $d$  is the dimensionality of the (presumed hypercubic) lattice and  $\mathcal{N}$  is the number of lattice sites, and from ferromagnetic fluctuations,

$$H_L = \frac{v_0}{2\mathcal{N}\hbar^2} \sum_{i,j} J_{ij} (1 - \eta_i \eta_j) \cdot \int d^d x \mathbf{L}^2(\mathbf{x}) - \frac{v_0}{4d\mathcal{N}\hbar^2} \sum_{i,j} J_{ij} |\mathbf{R}_i - \mathbf{R}_j|^2 \cdot \int d^d x (\partial_\mu L^a)^2 \quad . \quad (15.138)$$

Retaining only terms of order  $\mathbf{L}^2$  – and hence dropping terms of order  $(\nabla \mathbf{L})^2$  – we obtain the Hamiltonian,

$$H = \int d^d x \left\{ \frac{1}{2} \rho_s (\vec{\nabla} \hat{\mathbf{n}})^2 + \frac{1}{2} \chi^{-1} \mathbf{L}^2 \right\} \quad (15.139)$$

where the spin stiffness is given by

$$\rho_s \equiv -\frac{S^2}{2d\mathcal{N}v_0} \sum_{i,j} J_{ij} \eta_i \eta_j |\mathbf{R}_i - \mathbf{R}_j|^2 \quad (15.140)$$

and the inverse susceptibility is given by

$$\chi^{-1} \equiv \frac{v_0}{\mathcal{N}\hbar^2} \sum_{ij} J_{ij} (1 - \eta_i \eta_j) = \frac{v_0}{\hbar^2} \left[ \hat{J}(0) - \hat{J}(\mathbf{Q}) \right] \quad , \quad (15.141)$$

where  $\mathbf{Q} \equiv (\pi/a, \pi/a, \dots, \pi/a)$  is the zone corner wavevector. The dimensions of  $\rho_s$  and  $\chi$  are:

$$[\rho_s] = E \cdot L^{2-d} \quad ; \quad [\chi] = E \cdot T^2 \cdot L^{-d} \quad . \quad (15.142)$$

## 15.5.2 Geometric phase

The geometric phase contribution to the dimensionless action is written

$$\mathcal{A}_B = -S \sum_i \omega[\hat{\boldsymbol{\Omega}}_i(t)] = -S \sum_i \eta_i \omega \left[ \hat{\mathbf{n}}_i(t) + \eta_i \frac{v_0}{\hbar S} \mathbf{L}_i(t) \right] \quad . \quad (15.143)$$

We now expand in the notionally small quantity linear in  $\mathbf{L}_i$ , using the result of eqn. 15.88:

$$\begin{aligned} \mathcal{A}_B &= -S \sum_i \eta_i \omega[\hat{\mathbf{n}}_i] - S \int dt \sum_i \left( \frac{v_0}{\hbar S} \right) \mathbf{L}_i \cdot \frac{\partial \hat{\mathbf{n}}_i}{\partial t} \times \hat{\mathbf{n}}_i \\ &= -S \sum_i \eta_i \omega[\hat{\mathbf{n}}_i] - \frac{1}{\hbar} \int d^d x \int dt \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \hat{\mathbf{n}} \cdot \mathbf{L} \quad . \end{aligned} \quad (15.144)$$

### 15.5.3 Emergence of the nonlinear sigma model

Let's start with the quantum action obtained thus far,

$$\begin{aligned} \mathcal{A} = & -\frac{1}{\hbar} \int d^d x \int dt \left\{ \frac{1}{2} \rho_s (\vec{\nabla} \hat{\mathbf{n}})^2 + \frac{\mathbf{L}^2}{2\chi} + \mathbf{L} \cdot \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \hat{\mathbf{n}} \right. \\ & \left. + \frac{g_0 \mu_B}{\hbar S} \mathbf{H}_u \cdot \mathbf{L} + \frac{\hbar g_0 \mu_B}{v_0} \mathbf{H}_s \cdot \hat{\mathbf{n}} \right\} - S \sum_i \eta_i \omega[\hat{\mathbf{n}}_i] . \end{aligned} \quad (15.145)$$

We have included here an external field  $\mathbf{H}(\mathbf{x}, t)$  which has uniform ( $\mathbf{k} \approx 0$ ) and staggered ( $\mathbf{k} \approx \mathbf{Q}$ ) components  $\mathbf{H}_u$  and  $\mathbf{H}_s$ , respectively. Now let us integrate out  $\mathbf{L}$ . In order to do so, we must introduce a Lagrange multiplier field  $\lambda(\mathbf{x}, t)$  which enforces the local constraint  $\hat{\mathbf{n}} \cdot \mathbf{L} = 0$ . At each position  $\mathbf{x}$ , we must evaluate the functional integral

$$\begin{aligned} \mathcal{I} & \equiv \int \mathcal{D}\lambda(t) \int \mathcal{D}\mathbf{L}(t) \exp \left\{ -\frac{i}{\hbar} \int d^d x \int dt \left[ \frac{\mathbf{L}^2}{2\chi} + \mathbf{L} \cdot \left( \lambda \hat{\mathbf{n}} + \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \hat{\mathbf{n}} + \frac{g_0 \mu_B}{\hbar S} \mathbf{H}_u \right) \right] \right\} \\ & = \mathcal{I}_0 \int \mathcal{D}\lambda(t) \exp \left\{ \frac{i\chi}{2\hbar} \int d^d x \int dt \left( \lambda \hat{\mathbf{n}} + \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \hat{\mathbf{n}} + \frac{g_0 \mu_B}{\hbar S} \mathbf{H}_u \right)^2 \right\} \\ & = \tilde{\mathcal{I}}_0 \exp \left\{ \frac{i}{\hbar} \int d^d x \int dt \left[ \frac{1}{2} \chi \left( \frac{\partial \hat{\mathbf{n}}}{\partial t} \right)^2 + \frac{g_0 \mu_B \chi}{\hbar S} \mathbf{H}_u \cdot \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \hat{\mathbf{n}} + \frac{1}{2} \chi \left( \frac{g_0 \mu_B}{\hbar S} \right)^2 (\mathbf{H}_u \times \hat{\mathbf{n}})^2 \right] \right\} \end{aligned} \quad (15.146)$$

where  $\mathcal{I}_0$  and  $\tilde{\mathcal{I}}_0$  are independent of  $\mathbf{H}_u$  and  $\hat{\mathbf{n}}$ , and where we have suppressed the  $\mathbf{x}$  coordinate. The complete action functional, including the geometric phase term, is then

$$\begin{aligned} \mathcal{A} = & \frac{1}{\hbar} \int d^d x \int dt \left\{ \frac{1}{2} \chi \left( \frac{\partial \hat{\mathbf{n}}}{\partial t} \right)^2 - \frac{1}{2} \rho_s (\vec{\nabla} \hat{\mathbf{n}})^2 + \frac{g_0 \mu_B \chi}{\hbar S} \mathbf{H}_u \cdot \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \hat{\mathbf{n}} \right. \\ & \left. + \frac{1}{2} \chi \left( \frac{g_0 \mu_B}{\hbar S} \right)^2 (\mathbf{H}_u \times \hat{\mathbf{n}})^2 - \frac{g_0 \mu_B}{v_0} \mathbf{H}_s \cdot \hat{\mathbf{n}} \right\} - S \sum_i \eta_i \omega[\hat{\mathbf{n}}_i] . \end{aligned} \quad (15.147)$$

Dimensional analysis reveals the spin wave velocity  $c = \sqrt{\rho_s/\chi}$ . Defining  $x^0 = ct$ , we find that the quantum field theoretic action, excluding the geometric phase term, is

$$\begin{aligned} \mathcal{A} = & \frac{\rho_s}{2\hbar c} \int d^{d+1}x \left\{ (\partial_\mu n^a)(\partial^\mu n^a) + \frac{2g_0 \mu_B}{\hbar c S} \mathbf{H}_u \cdot \frac{\partial \hat{\mathbf{n}}}{\partial x^0} \times \hat{\mathbf{n}} \right. \\ & \left. + \left( \frac{g_0 \mu_B}{\hbar c S} \right)^2 (\mathbf{H}_u \times \hat{\mathbf{n}})^2 - \frac{2g_0 \mu_B}{\rho_s v_0} \mathbf{H}_s \cdot \hat{\mathbf{n}} \right\} - S \sum_i \eta_i \omega[\hat{\mathbf{n}}_i] . \end{aligned}$$

where we adopt a Minkowski (+, −, ..., −) metric. The Euclidean version is

$$\begin{aligned} \mathcal{A}^E = & \frac{\rho_s}{2\hbar c} \int d^{d+1}x \left\{ (\partial_\mu n^a)(\partial_\mu n^a) + \frac{2ig_0 \mu_B}{\hbar c S} \mathbf{H}_u \cdot \frac{\partial \hat{\mathbf{n}}}{\partial x^0} \times \hat{\mathbf{n}} \right. \\ & \left. - \left( \frac{g_0 \mu_B}{\hbar c S} \right)^2 (\mathbf{H}_u \times \hat{\mathbf{n}})^2 + \frac{2g_0 \mu_B}{\rho_s v_0} \mathbf{H}_s \cdot \hat{\mathbf{n}} \right\} + iS \sum_i \eta_i \omega[\hat{\mathbf{n}}_i] . \end{aligned} \quad (15.148)$$

Notice the factor of  $i$  in the coefficient of the second term. To maximize the weight  $\exp(-\mathcal{A}^E)$ , the third term inside the brackets should be as large as possible. This favors a *spin flop* in which the Néel vector lies perpendicular to the (uniform) applied magnetic field  $\mathbf{H}_u$ .

The *coupling constant* for the nonlinear sigma model is defined to be

$$g = \frac{\hbar c}{\rho_s} = \frac{\hbar}{\sqrt{\rho_s \chi}} = \frac{\sqrt{2d} v_0}{aS} \left( \frac{\sum_{i,j} J_{ij} (1 - \eta_i \eta_j)}{\sum_{i,j} J_{ij} (-\eta_i \eta_j) |\mathbf{R}_i - \mathbf{R}_j|^2 / a^2} \right)^{1/2} . \quad (15.149)$$

For a nearest neighbor model on a  $d$ -dimensional cubic lattice, we have<sup>6</sup>

$$g = \frac{2\sqrt{d} a^{d-1}}{S} . \quad (15.150)$$

#### 15.5.4 Continuum limit of the geometric phase: $d = 1$

In one space dimension, we have

$$\sum_j (-1)^j \omega[\hat{\mathbf{n}}_j] = \omega[\hat{\mathbf{n}}_0] - \omega[\hat{\mathbf{n}}_1] + \omega[\hat{\mathbf{n}}_2] - \dots = \frac{1}{2} \int_0^L dx \frac{\partial \omega}{\partial x} . \quad (15.151)$$

We now invoke eqn. 15.88, which says

$$\delta \omega = \int_0^T dt \epsilon_{abc} \dot{n}^b n^c \delta n^a , \quad (15.152)$$

to obtain the beautiful result,

$$\mathcal{A}_B = -S \sum_j (-1)^j \omega[\hat{\mathbf{n}}_j] = \frac{1}{2} S \int dx \int dt \hat{\mathbf{n}} \cdot \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \frac{\partial \hat{\mathbf{n}}}{\partial x} \equiv 2\pi S Q_{tx} , \quad (15.153)$$

where  $Q_{tx}$  is an integer topological invariant, known as the *Pontrjagin index* of the field  $\hat{\mathbf{n}}(x, t)$ :

$$Q_{tx} = \frac{1}{8\pi} \int d^2x \epsilon^{\mu\nu} \epsilon_{abc} n^a \partial_\mu n^b \partial_\nu n^c , \quad (15.154)$$

where  $x^0 = ct$  as before.  $Q_{tx}$  measures the winding of the field  $\hat{\mathbf{n}}(x, t)$  over the unit sphere. To see it is an integer, change variables from local coordinates  $(n^b, n^c)$  to  $(\xi_0, \xi_1)$  in the vicinity of  $\hat{\mathbf{n}}$ . The differential surface area element projected along  $n^a$  is

$$d\Sigma_a = \frac{1}{2} \epsilon^{\mu\nu} \epsilon_{abc} \frac{\partial n^b}{\partial \xi^\mu} \frac{\partial n^c}{\partial \xi^\nu} d^2\xi \quad (15.155)$$

<sup>6</sup>Take care not to confuse the coupling  $g$  with the  $g$ -factor  $g_0$ .

and changing variables from  $(x^0, x^1)$  to  $(\xi^0, \xi^1)$ , we obtain

$$Q_{tx} = \frac{1}{4\pi} \int_{S_{\text{int}}^2} d^2\xi \quad , \quad (15.156)$$

which is manifestly an integer.

Put another way, think of  $\hat{n}(x, t)$  as a rubber band draped over the surface of a sphere. As time evolves from 0 to  $T$ , the configuration of the rubber band changes, but if the configuration itself is periodic, *i.e.*  $\hat{n}(x, 0) = \hat{n}(x, T)$ , The Pontrjagin index measures the number of times the rubber band winds around the sphere. Configurations of  $\hat{n}(x, t)$  which yield a nonzero value of  $Q_{tx}$  are known as *skyrmions*. An example of a skyrmion configuration on the two-dimensional  $(x, y)$  (or  $(x, t)$ ) plane is obtained by identifying the vector  $\hat{n}(x, y)$  with the (inverse) stereographically projected position  $(x, y)$ . Put another way, we set

$$\frac{v}{u} = \tan(\theta/2) e^{i\phi} \equiv (x + iy)/a \quad , \quad (15.157)$$

where  $a$  is an arbitrary length scale. This (*exercise!*) is equivalent to

$$n_x = \frac{2ax}{a^2 + x^2 + y^2} \quad , \quad n_y = \frac{2ay}{a^2 + x^2 + y^2} \quad , \quad n_z = \frac{a^2 - x^2 - y^2}{a^2 + x^2 + y^2} \quad . \quad (15.158)$$

This skyrmion has Pontrjagin index  $Q_{xy} = 1$ .

Thermodynamic properties are derived from the Euclidean action,

$$\mathcal{A}_{d=1}^{\text{E}} = 2\pi i S Q_{tx} + \frac{\rho_s}{2\hbar c} \int d^2x (\vec{\nabla} \hat{n})^2 \quad . \quad (15.159)$$

The effect of the geometric phase term, then, is quite simple and in fact discrete:

$$e^{2\pi i S Q_{tx}} = \begin{cases} +1 & \text{if } S \in \mathbf{Z} \\ (-1)^{Q_{tx}} & \text{if } S \in \mathbf{Z} + \frac{1}{2} \end{cases} \quad . \quad (15.160)$$

Thus, for integer  $S$ , the geometric phase term always contributes a factor of unity, and the full quantum field theoretic action is that of the two-dimensional O(3) model, also called the nonlinear sigma model. For half-odd integer  $S$ , space-time configurations with even and odd Pontrjagin index destructively interfere with each other.

What have we learned? First of all, we conclude that antiferromagnetic Heisenberg chains generically fall into two classes: those with integer spin and those with half-odd integer spin. The field theory for the first class is simply that of the classical O(3) model in two dimensions. The Hohenberg-Mermin-Wagner theorem precludes any spontaneous breaking of the continuous O(3) symmetry in  $d = 2$  at any finite value of  $\rho_s$ . The system has a gap, and correlation functions decay exponentially, up to power law corrections, *viz.*

$$\langle \Psi_0 | \mathbf{S}_0 \cdot \mathbf{S}_j | \Psi_0 \rangle \simeq (-1)^j |j|^{-1/2} \exp(-|j|/\xi) \quad , \quad (15.161)$$



where the correlation length  $\xi$ , in units of the lattice spacing  $a$ , is a function of the dimensionless quantity  $\rho_s/\hbar c$ .

For the second class – the half-odd integer antiferromagnetic chains – the field theory includes the so-called ‘ $\theta$ -term’,

$$\mathcal{A}_\theta = \frac{\theta}{4\pi} \int dx \int dt \hat{\mathbf{n}} \cdot \frac{\partial \hat{\mathbf{n}}}{\partial t} \times \frac{\partial \hat{\mathbf{n}}}{\partial x} \quad , \quad (15.162)$$

with  $\theta = 2\pi S = \pi \bmod 2\pi$ . While no exact solution to the field theory with the  $\theta$ -term is yet known, we nonetheless conclude that all half-odd integer antiferromagnetic chains behave equivalently, since they all map onto the same model. Since the  $S = \frac{1}{2}$  Heisenberg antiferromagnetic chain is known, from Bethe’s *Ansatz*, to possess a disordered ground state with gapless excitations and power law correlations,  $\langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle \sim (-1)^j/|j|$  (up to logarithmic corrections), we conclude that the same is true for the  $S = \frac{3}{2}, \frac{5}{2}, \text{etc.}$  spin chains.

### 15.5.5 The geometric phase in higher dimensions

So long as the Néel field  $\hat{\mathbf{n}}(x, t)$  is a smooth function of space and time, there are no interesting topological terms in the field theory in more than one space dimension. The reason is trivial. Consider a  $d$ -dimensional system as a network of parallel one-dimensional chains. Call the longitudinal (chain) coordinate  $x$ . For each set of transverse coordinates  $\mathbf{R}_\perp$ , one can define the integer Pontrjagin index  $Q_{tx}(\mathbf{R}_\perp)$ . The geometric phase term in the action is then given by

$$\mathcal{A}_B = S \sum_i \eta_i \omega[\hat{\mathbf{n}}_i] = S \sum_{\mathbf{R}_\perp} \eta_{\mathbf{R}_\perp} Q_{tx}(\mathbf{R}_\perp) = 0 \quad , \quad (15.163)$$

where the last equality follows from the assumed smoothness of  $\hat{\mathbf{n}}(x, t)$ , which requires that  $Q_{tx}(\mathbf{R}_\perp)$  be independent of  $\mathbf{R}_\perp$ , since a smooth integer-valued function must be a constant!

When the smoothness constraint is relaxed, however, the geometric phase term can play an important role. For a two-dimensional antiferromagnet, there exist topology-changing instanton for which  $\Delta Q_{xy} = \pm 1$ . Such field configurations are called ‘hedgehogs’, because the direction of the field  $\hat{\mathbf{n}}(t, x, y)$  points radially outward from the center of the hedgehog. For quantum-disordered two-dimensional antiferromagnets (*i.e.* small  $\rho_s$ ), Haldane argued that geometrical phase considerations associated with the presence of hedgehogs would distinguish not only between integer and half-odd integer  $S$  on the square lattice, but between even and odd integer  $S$  as well.

## 15.6 Large- $N$ Techniques

The basic idea behind large- $N$  approaches is to extend the global symmetry group of some physical model from *e.g.*  $O(3)$ ,  $SU(2)$ , *etc.* to a larger group, such as  $O(N)$ ,  $SU(N)$ , or  $Sp(N)$ . If the

extension is done in a certain way, the resultant model can be solved exactly in the  $N \rightarrow \infty$  limit.  $N$  plays the role of  $1/\hbar$ , so  $N \rightarrow \infty$  is a classical limit of sorts, with no quantum fluctuations. Furthermore, one can derive a systematic diagrammatic expansion in powers of  $1/N$ , which can be used to investigate properties at finite  $N$ .

We shall barely scratch the surface of this subject. My aim here is to guide you through a large- $N$  calculation for the nonlinear sigma model.

### 15.6.1 $1/N$ expansion for an integral

To begin, consider the one-dimensional integral,

$$\mathcal{I} = \int_{-\infty}^{\infty} dx e^{-Nf(x)} \quad , \quad (15.164)$$

where  $f(x)$  is some function and  $N$  is large. Clearly the integral is dominated by values of  $x$  near the minimum of  $f(x)$ . Suppose a unique global minimum exists at  $x = x_c$ . We can then write

$$\begin{aligned} \mathcal{I} &= e^{-Nf(x_c)} \int_{-\infty}^{\infty} du e^{-\frac{1}{2}Nf''(x_c)u^2} e^{-\frac{1}{6}Nf'''(x_c)u^3} e^{-\frac{1}{24}Nf''''(x_c)u^4} \dots \\ &= e^{-Nf(x_c)} \int_{-\infty}^{\infty} du e^{-\frac{1}{2}Nf''(x_c)u^2} \left\{ 1 - \frac{1}{6}Nf'''(x_c)u^3 - \frac{1}{24}Nf''''(x_c)u^4 + \dots \right\} \\ &= \left( \frac{2\pi}{Nf''(x_c)} \right)^{1/2} e^{-Nf(x_c)} \left\{ 1 - \frac{1}{24}Nf''''(x_c)\langle u^4 \rangle + \dots \right\} \quad . \end{aligned} \quad (15.165)$$

Thus, we have derived a  $1/N$  expansion for the integral:

$$-\ln \mathcal{I} = \underbrace{Nf(x_c)}_{\mathcal{O}(N^1)} + \underbrace{\frac{1}{2} \ln \left( \frac{Nf''(x_c)}{2\pi} \right)}_{\mathcal{O}(N^0)} + \underbrace{\frac{1}{8N} \frac{f''''(x_c)}{[f''(x_c)]^2}}_{\text{corrections } \mathcal{O}(N^{-1})} + \mathcal{O}(N^{-2}) \quad . \quad (15.166)$$

### 15.6.2 Large- $N$ theory of the nonlinear sigma model

Recall the Euclidean action for the  $O(3)$  nonlinear sigma model,

$$\mathcal{A}_E = \frac{\rho_s}{2\hbar c} \int d^d x \int_0^{L_0} dx^0 (\partial_\mu n^a)^2 \quad , \quad (15.167)$$

where  $\hat{\mathbf{n}} = (n^x, n^y, n^z)$  is a three-component unit vector and  $L_0 = \hbar c/k_B T$ . In the case of Haldane's derivation of the sigma model action for quantum antiferromagnets,  $\hat{\mathbf{n}}(x)$  is physically the Néel field, which varies slowly from site to site even though the local magnetization itself oscillates from one sublattice to the next.<sup>7</sup> It should be emphasized, though, that the  $D$ -dimensional nonlinear sigma model also describes the finite temperature phase transition of an isotropic  $D$ -dimensional ferromagnet.

Quantum mechanics is irrelevant at finite temperature, since the imaginary time variable is bounded:  $0 \leq \tau \leq \hbar\beta$ . At a critical point, the spatial correlation length diverges as  $\xi(T) \sim |T - T_c|^{-\nu}$ , and the temporal correlation length (or correlation time) diverges along with  $\xi$ , as  $\xi_\tau \sim \xi^z$ . Here,  $\nu$  is the correlation length exponent and  $z$  the dynamic critical exponent. With  $\hbar\beta$  finite, however, sufficiently close to  $T_c$  the correlation time exceeds the thickness  $\hbar\beta$  of the temporal 'slab', hence the degrees of freedom at a particular location in space are 'locked' as a function of imaginary time. Finite  $T$  second order transitions of a  $d$ -dimensional quantum system are therefore described by a  $d$ -dimensional action.<sup>8</sup> At zero temperature, though, the temporal slab is infinitely thick, and one cannot ignore temporal fluctuations. The action is then for a  $(d + 1)$ -dimensional system.

It is perhaps worth emphasizing that the continuum effective action for the Heisenberg *ferromagnet* is given by

$$\mathcal{A}_{\text{FM}} = \int d^d x \int_0^{\hbar\beta} d\tau \left\{ iS v_0^{-1} \mathbf{A}(\hat{\mathbf{n}}) \cdot \frac{\partial \hat{\mathbf{n}}}{\partial \tau} + \frac{1}{2} \rho_s (\vec{\nabla} \hat{\mathbf{n}})^2 \right\} \quad (15.168)$$

where  $v_0$  is the unit cell volume, and

$$\rho_s = \frac{S^2}{4dv_0} \sum_{\mathbf{R}} J(\mathbf{R}) \mathbf{R}^2 \quad . \quad (15.169)$$

Note the difference between this and the effective action of the antiferromagnet, in which space and time appear symmetrically. The effective (low-energy) theory for the antiferromagnet possesses a 'Lorentz invariance' where the speed of light is replaced by the spin wave velocity  $c = \sqrt{\rho_s/\chi}$ .

Returning to the nonlinear sigma model, the partition function is given by the functional integral

$$Z = e^{-F/k_B T} = \int_{\hat{\mathbf{n}}^2=1} \mathcal{D}\hat{\mathbf{n}}(x) e^{-\mathcal{A}_{\text{E}}[\hat{\mathbf{n}}]} \quad . \quad (15.170)$$

<sup>7</sup>The notation I adopt here is that  $(d + 1)$ -dimensional vectors are denoted as  $x \equiv (x^0, \mathbf{x})$ .

<sup>8</sup>Note that this *does not* say that quantum mechanics has no effect whatsoever at finite temperature. Indeed, the partition function for the quantum and classical Heisenberg models will be different. What *is* true is that the *critical properties* at a finite temperature *second order* transition are not affected by quantum mechanics.

The extension of the O(3) model to one with an O( $N$ ) symmetry is trivial. Simply replace the 3-component unit vector  $(n_x, n_y, n_z)$  by an  $N$ -component one,  $\mathbf{n} = (n_1, n_2, \dots, n_N)$ . How do we generalize the unit length constraint to general  $N$ ? Let us write the constraint as  $\mathbf{n}^2(x) = qN$ , where the parameter  $q$  is as yet undetermined. We can envisage two natural extensions to general  $N$ :

- Maintain  $\mathbf{n}^2 = 1$ , i.e. take  $q = N^{-1}$ .
- Fix  $q$  and let  $N$  vary. The length of  $\mathbf{n}$  then increases with  $N$ .

It turns out that it is the second of these schemes which generates a proper  $1/N$  expansion, as we shall soon see.

To enforce the length constraint, we insert into the functional integral a  $\delta$ -function  $\delta(\hat{\mathbf{n}}^2 - qN)$  at every space-time point. We write the  $\delta$ -function as

$$\delta(y) = \int_{-i\infty}^{i\infty} d\lambda e^{-\lambda y} \quad , \quad (15.171)$$

where the integration contour runs along the imaginary axis, from  $-i\infty$  to  $+i\infty$ . The partition function is then expressed as a double functional integral over the fields  $\hat{\mathbf{n}}(x)$  and  $\lambda(x)$ ,

$$Z = \int \mathcal{D}[\mathbf{n}(x), \lambda(x)] e^{-\tilde{\mathcal{A}}_E[\mathbf{n}, \lambda]} \quad , \quad (15.172)$$

where

$$\tilde{\mathcal{A}}_E = \int d^{d+1}x \left\{ \frac{1}{2g} (\partial_\mu n^a)^2 + \lambda (\mathbf{n}^2 - qN) \right\} \quad . \quad (15.173)$$

For convenience we have defined the coupling

$$g \equiv \frac{\hbar c}{\rho_s} = \frac{\hbar}{\sqrt{\chi \rho_s}} \quad . \quad (15.174)$$

The dimensions of  $g$  are  $[g] = L^{d-1}$ .

We now integrate out the  $n^a(x)$  fields, which are quadratic in  $\tilde{\mathcal{A}}_E$ . Writing

$$\tilde{\mathcal{A}}_E = \frac{1}{2} \int d^{d+1}x \int d^{d+1}x' n^a(x) K(x, x') n^a(x') - qN \int d^{d+1}x \lambda(x) \quad (15.175)$$

with

$$K(x, x') = -\frac{\rho_s}{\hbar c} \frac{\partial}{\partial x^\mu} \delta(x - x') \frac{\partial}{\partial x'^\mu} + 2\lambda \delta(x - x') \quad , \quad (15.176)$$

the partition function can be written in terms of an effective free energy which is a function of the field  $\lambda(x)$  alone:

$$Z = \int \mathcal{D}\lambda(x) e^{-NF_{\text{eff}}[\lambda]/k_{\text{B}}T} \quad (15.177)$$

where

$$\begin{aligned} e^{-NF_{\text{eff}}[\lambda]/k_{\text{B}}T} &= \int \mathcal{D}\mathbf{n}(x) e^{-\tilde{\mathcal{A}}_{\text{E}}[\mathbf{n}(x), \lambda(x)]} \\ &= (\det K)^{-N} \exp \left\{ qN \int d^{d+1}x \lambda(x) \right\} . \end{aligned} \quad (15.178)$$

Thus, the effective free energy is

$$F_{\text{eff}}[\lambda]/k_{\text{B}}T = \ln \det K - q \int d^{d+1}x \lambda(x) , \quad (15.179)$$

where the determinant of the integral operator  $K$  is, as always, defined by the product of its eigenvalues,

$$\ln \det K = \prod_n \zeta_n . \quad (15.180)$$

The eigenvalue equation is

$$\int d^{d+1}x' K(x, x') \psi_n(x') = \zeta_n \psi_n(x) . \quad (15.181)$$

We can now see why keeping  $q$  finite as  $N \rightarrow \infty$  generates a true  $1/N$  expansion. Had we instead taken  $n^2 = 1$ , we would have  $q = 1/N$  and the effective free energy  $F_{\text{eff}}[\lambda]$  would not be independent of  $N$ .

### Solution of the $N \rightarrow \infty$ theory

When  $N \rightarrow \infty$  the functional integral is dominated by the saddle point in the action. Before we solve for this saddle point, let us slightly extend our model to include a coupling to a magnetic field. The augmented action is then

$$\tilde{\mathcal{A}}_{\text{E}} = \int d^{d+1}x \left\{ \frac{1}{2g} (\partial_{\mu} n^a)^2 + \lambda (n^a n^a - qN) - \sqrt{N} h^a n^a \right\} . \quad (15.182)$$

The  $\sqrt{N}$  factor preceding  $\mathbf{h} \cdot \mathbf{n}$  ensures that the action will be proportional to  $N$  when  $|\mathbf{h}|$  is of  $\mathcal{O}(N^0)$ . In the case of the antiferromagnet, where  $\hat{\mathbf{n}}$  is the Néel field,  $\mathbf{h}$  corresponds to the  $q = \pi/a$  (zone corner) component of the physical magnetic field, *i.e.* a sublattice-staggered magnetic field. This is of course quite unphysical, however our purpose in introducing  $\mathbf{h}$  is not to

investigate the effects of an external field *per se*, but rather as an artifice by which we can couple to any condensate, as we shall see presently.

To find the saddle point of  $F_{\text{eff}}[\lambda]$ , we should set its functional variation with respect to  $\lambda(x)$  to zero. We will assume that the saddle point occurs for real, constant  $\lambda$ . We will justify this by presenting such a solution to the equation  $\delta F_{\text{eff}} = 0$ . Note that the saddle point lies off the integration contour for  $\lambda(x)$ , which runs along the imaginary axis.

When  $\lambda$  is constant, the model may be solved by Fourier transform. We write

$$n^a(x) = \frac{1}{\sqrt{L_0 V}} \sum_k \hat{n}^a(k) e^{ik \cdot x} \quad (15.183)$$

with

$$L_0 = \beta \hbar c \quad , \quad V = L_1 \cdots L_d \quad , \quad k = \left( \frac{2\pi j_0}{L_0}, \frac{2\pi j_1}{L_1}, \dots, \frac{2\pi j_d}{L_d} \right) \quad . \quad (15.184)$$

Expressed in terms of the Fourier modes,

$$\left\{ \begin{array}{l} n^a(x) \\ h^a(x) \end{array} \right\} \equiv \frac{1}{\sqrt{V L_0}} \sum_k \left\{ \begin{array}{l} \hat{n}^a(k) \\ \hat{h}^a(k) \end{array} \right\} e^{ik \cdot x} \quad , \quad (15.185)$$

the Euclidean action is

$$\tilde{\mathcal{A}}_E = \sum_{a=1}^N \sum_k \left\{ \left( \lambda + \frac{k^2}{2g} \right) |\hat{n}^a(k)|^2 - \sqrt{N} \hat{h}_a^*(k) \hat{n}^a(k) \right\} - q N V L_0 \lambda \quad . \quad (15.186)$$

We now integrate out the  $\{\hat{n}^a(k)\}$ , yielding an effective free energy function  $F_{\text{eff}}(\lambda)$ :

$$f(\lambda) \equiv \frac{F_{\text{eff}}(\lambda)}{N \hbar c V} = -q \lambda + \frac{1}{2L_0 V} \sum_k \ln \left( \lambda + \frac{k^2}{2g} \right) - \frac{1}{2L_0 V} \sum_k \frac{\hat{h}^a(k) \hat{h}^a(-k)}{\left( \lambda + \frac{k^2}{2g} \right)} \quad . \quad (15.187)$$

The order parameter  $m$ , which is the static Néel field in the case of the antiferromagnet and the static magnetization in the case of the ferromagnet, is obtained by differentiating the free energy with respect to the  $q = 0$  Fourier component of the field  $\hat{h}^a(k)$ . We therefore obtain

$$m = \frac{\langle \mathbf{n} \rangle}{\sqrt{N}} = -\frac{1}{N L_0 V} \frac{\partial (N F_{\text{eff}} / k_B T)}{\partial \mathbf{h}} = -\frac{\partial f}{\partial \mathbf{h}} = \frac{\mathbf{h}}{2\lambda} \quad , \quad (15.188)$$

since  $\hat{h}(0) = \sqrt{L_0 V} \mathbf{h}$ .

To find the saddle point in  $\lambda$ , we set  $\partial f / \partial \lambda = 0$ , yielding

$$q = m^2 + \frac{g}{L_0 V} \sum_k \frac{1}{k^2 + 2g\lambda} \quad . \quad (15.189)$$

In the absence of an external field, we also have The second mean field equation,

$$2\lambda \mathbf{m} = \mathbf{h} = 0 \quad . \quad (15.190)$$

This requires either (i)  $\lambda = 0$  or (ii)  $\mathbf{m} = 0$ .

We now explore the solution to these equations as we vary dimensionality and temperature.

- $d = 1, T = 0$ : In this case the integral is infrared divergent when  $\lambda = 0$ . The mean field equation can always be solved with  $\mathbf{m} = 0$  for some finite  $\lambda$ :

$$q = \int \frac{d^2k}{(2\pi)^2} \frac{1}{2\lambda + \frac{k^2}{g}} = \frac{g}{4\pi} \ln \left( 1 + \frac{\Lambda^2}{2g\lambda} \right) \quad , \quad (15.191)$$

yielding

$$\lambda(g) = \frac{\Lambda^2/2g}{\exp(4\pi q/g) - 1} \quad , \quad (15.192)$$

which monotonically decreases on  $g \in [0, \infty]$  from  $\lambda(0) = \Lambda^2/8\pi q$  to  $\lambda(\infty) = 0$ .

- $d > 1, T = 0$ : In this case there exists a quantum critical point at  $g = g_c$ . The gap  $\lambda$  vanishes for  $g \leq g_c$ . To find  $g_c$ , set

$$q = g_c \int \frac{d^{d+1}k}{(2\pi)^{d+1}} \frac{1}{k^2} = \frac{g_c}{(2\pi)^{d+1}} \cdot \frac{\Lambda^{d-1}}{d-1} \cdot \begin{cases} \Omega_{d+1} & \text{scheme I} \\ \pi\Omega_d & \text{scheme II} \end{cases} \quad , \quad (15.193)$$

where  $\Omega_d$  is the area of the  $d$ -dimensional unit sphere:

$$\Omega_d = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})} \quad . \quad (15.194)$$

The cutoff is taken to be isotropic in both frequency and momentum (scheme I) or isotropic in momentum only (scheme II). In scheme II, the integral over the frequency component  $k_0$  extends over the range  $(-\infty, \infty)$ , which is appropriate since the imaginary time variable is not quantized on a lattice. This gives us an equation for the critical coupling  $g_c$ . The cutoff  $\Lambda$  is proportional to  $a^{-1}$ , and it is convenient to write  $\Lambda = \zeta\pi/a$ , where  $\zeta$  is a dimensionless constant and  $a$  is the lattice spacing.

Recall that Haldane's mapping for the cubic lattice Heisenberg model resulted in an  $O(3)$  nonlinear sigma model with coupling  $g = 2\sqrt{d} a^{d-1}/S$ . The critical value for the spin quantum number  $S_c$  is then found to be

$$S_c = \frac{\sqrt{d}}{d-1} \cdot \frac{\zeta^{d-1}}{2^d \pi^2 q} \cdot \begin{cases} \Omega_{d+1} & \text{scheme I} \\ \pi\Omega_d & \text{scheme II} \end{cases} \quad , \quad (15.195)$$

For  $d = 2$  and  $q = N^{-1} = \frac{1}{3}$ , one finds  $S_c = 1.35 \zeta$  (scheme I) or  $S_c = 2.12 \zeta$  (scheme II). Depending on the value of  $\zeta$ , then, the critical  $S$  may be either smaller or greater than the smallest value permitted by quantum mechanics, *i.e.*  $S = \frac{1}{2}$ . If  $S_c < \frac{1}{2}$ , then we conclude the model is Néel-ordered at zero temperature. Indeed numerical work convincingly shows that the ground state for  $S = \frac{1}{2}$  is Néel-ordered, and rigorous proofs exist which show that long-ranged Néel order exists for  $S \geq 1$ .

One might suspect, given eqn. 15.149, that by extending the range of the interactions one can push  $g$  above  $g_c$  and obtain a quantum-disordered ‘spin-liquid’ ground state for the  $S = \frac{1}{2}$  antiferromagnet on a square lattice. For example, if one includes next-nearest neighbor antiferromagnetic coupling  $J_2$  as well as nearest neighbor antiferromagnetic coupling  $J_1$ , one has

$$g = \frac{2\sqrt{d} a^{d-1}}{S} \cdot \frac{1}{\sqrt{1 - 2J_2/J_1}} \quad , \quad (15.196)$$

which is increased above its value when  $J_2 = 0$ . In fact, the search for spin liquid states has been an arduous one. On the square lattice, one generally finds that frustrating further-neighbor couplings push the system into another ordered state, for example one with four sublattice antiferromagnetic order. On lattices which are highly geometrically frustrated, such as the Kagomé and pyrochlore lattices, the  $S = \frac{1}{2}$  antiferromagnet is generally believed to have a quantum-disordered spin liquid ground state, *i.e.* the ground state has no long-ranged order and breaks no lattice translation or point group symmetries.

- $d > 2, T > 0$ : In this case there is a finite temperature phase transition. Defining the Matsubara wavevectors  $\kappa_n \equiv 2\pi n/L_0$ , we use the result

$$\frac{1}{L_0} \sum_{\kappa_n} H(-i\kappa_n) = \frac{H(0)}{L_0} + \int_{-\infty}^{\infty} \frac{d\kappa}{\pi} \frac{\text{Im } H(\kappa + i0^+)}{\exp(\kappa L_0) - 1} \quad (15.197)$$

to obtain the finite temperature mean field equation,

$$q = m^2 + g \int \frac{d^d k}{(2\pi)^d} \left\{ \frac{2/L_0}{k^2 + 2g\lambda} + \frac{\text{ctnh}(\frac{1}{2}L_0\sqrt{k^2 + 2g\lambda})}{\sqrt{k^2 + 2g\lambda}} \right\} \quad (15.198)$$

The equation for  $T_c$  is obtained by setting  $\lambda = m^2 = 0$ :

$$q = g \int \frac{d^d k}{(2\pi)^d} \left\{ \frac{2}{L_0 k^2} + \frac{1}{k} \text{ctnh}(\frac{1}{2}kL_{0,c}) \right\} \quad , \quad (15.199)$$

which is to be solved for  $T_c = \hbar c/k_B L_{0,c}$ , assuming  $g < g_c$ , *i.e.* that the  $T = 0$  (ground) state is ordered.



### 15.6.3 Correlation functions

The correlation functions are obtained via

$$\langle \hat{n}^a(k) \hat{n}^b(-k) \rangle_c = -L_0 V \frac{\partial^2 f}{\partial \hat{h}^a(-k) \partial \hat{h}^b(k)} = \frac{g}{k^2 + 2g\lambda} \delta^{ab} \quad (15.200)$$

hence the full correlator is given by

$$\begin{aligned} C_{ab}(x) &\equiv \langle n^a(0) n^b(x) \rangle = m^a m^b + \frac{g}{L_0 V} \sum_k \frac{e^{ik \cdot x}}{k^2 + 2g\lambda} \delta^{ab} \\ &= m^a m^b + g \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} e^{ik_0 x^0} \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik \cdot x}}{k_0^2 + \mathbf{k}^2 + 2g\lambda} \quad , \end{aligned} \quad (15.201)$$

where in the second line we take the thermodynamic limit, set  $T \rightarrow 0$ , and adopt cutoff scheme II, appropriate for lattice systems. In the latter case, at large distances we obtain the Ornstein-Zernike form,

$$C_{ab}(x) - C_{ab}(\infty) \sim \frac{e^{-|x|/\xi}}{|x|^{d/2}} \delta^{ab} \quad , \quad (15.202)$$

with  $\xi = (2g\lambda)^{-1/2}$ . At the quantum critical point, where  $\lambda$  vanishes, one finds  $C(x) \sim |x|^{1-d}$ .