7
Large Orders in Perturbation Theory

7.1 Generalities

We can use instanton methods to obtain the size of the terms in large orders of perturbation theory. We will first consider particle quantum mechanics [21] and then generalize to quantum field theory. The general idea concerns actions of the form

$$S\left(\phi\right) = \int d^d x \left(\frac{1}{2} \partial_\mu \phi \partial_\mu \phi + \frac{g}{(2N)!} \phi^{2N} \right) \tag{7.1}$$

with $N = \frac{d}{d-2}$. With

$$\mathcal{I}(g) = \int \mathcal{D}\phi\, e^{-\frac{S(\phi)}{\hbar}} = \sum_k \mathcal{I}_k g^k \tag{7.2}$$

we have from Cauchy's formula

$$\mathcal{I}_k = \frac{1}{2\pi i} \oint dg \left(\frac{\mathcal{I}(g)}{g^{k+1}} \right), \tag{7.3}$$

where the integral is over a contour containing the origin. For large k we want to perform this integral by Gaussian approximation about a critical point in ϕ and g. The critical point must satisfy the equations of motion, $\bar{h} = 1$,

$$0 = \frac{\partial}{\partial g} \frac{e^{-\frac{S(\phi,g)}{\hbar}}}{g^k} \Rightarrow \frac{k}{g} = -\frac{1}{(2N)!} \int d^d x \phi^{2N} \tag{7.4}$$

and the usual equation for ϕ

$$\partial_\mu \partial^\mu \phi = \frac{g}{(2N-1)!} \phi^{(2N-1)}. \tag{7.5}$$

Changing the scale

$$\phi \to (-g)^{-\frac{1}{2N-2}} \psi \tag{7.6}$$

gives

$$\frac{k}{g} = -\frac{1}{(2N)!} (-g)^{-\frac{N}{N-1}} \int d^d x \psi^{2N}, \tag{7.7}$$

which implies

$$(2N)! \frac{k}{\int d^d x \psi^{2N}} = (-g)^{-\frac{N}{N-1}+1} = (-g)^{-\frac{1}{N-1}}, \tag{7.8}$$

which in turn means

$$-g \sim \frac{1}{k^{N-1}}. \tag{7.9}$$

The other equation is simply

$$(-g)^{-\frac{1}{2N-2}} \partial_\mu \partial^\mu \psi = g \frac{\psi^{2N-1}}{(2N-1)!} (-g)^{-\frac{2N-1}{2N-2}}, \tag{7.10}$$

which should have a solution with

$$\int d^d x \psi^{2N} < \infty. \tag{7.11}$$

We find such a critical point in various examples, and then perform the integrals by Gaussian approximation.

7.2 Particle Mechanics

In particle quantum mechanics we consider the Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^{n} p_i^2 + \frac{1}{2} \sum_{i=1}^{n} x_i^2 + g \left(\sum_{i=1}^{n} x_i^2 \right)^N, \tag{7.12}$$

which describes n anharmonic oscillators which interact with each other. Then

$$\lim_{\beta \to \infty} -\frac{1}{\beta} \ln \left(\frac{\mathrm{tr}\left(e^{-\beta H}\right)}{\mathrm{tr}\left(e^{-\beta H_0}\right)} \right) = \lim_{\beta \to \infty} -\frac{1}{\beta} \ln \left(\frac{e^{-\beta \mathcal{E}} + \cdots}{e^{-\beta \mathcal{E}_0} + \cdots} \right) = \mathcal{E} - \mathcal{E}_0, \tag{7.13}$$

where $\mathcal{E}$ and $\mathcal{E}_0$ are the ground-state energy of the system and the corresponding free system. The ratio of the traces can be expressed as a path integral

$$\frac{\mathrm{tr}\left(e^{-\beta H}\right)}{\mathrm{tr}\left(e^{-\beta H_0}\right)} = \mathcal{N} \int_{periodic} \mathcal{D}\vec{x}(\tau) e^{-\int_0^\beta d\tau \left(\frac{1}{2}\dot{\vec{x}}^2 + \frac{1}{2}\vec{x}^2 + g|\vec{x}|^N \right)}. \tag{7.14}$$

$\mathcal{N}$ is chosen so that the ratio is equal to 1 for $g = 0$. Periodic $\vec{x}(\tau)$ converts the path integral into a trace. The term of order k is extracted via the Cauchy theorem. This integral corresponds to the integral in Equation (7.2).

For particle quantum mechanics, however, we can actually perform the g integration exactly,

$$\frac{1}{2\pi i} \oint dg \frac{e^{-g \int_o^\beta d\tau |\vec{x}|^{2N}}}{g^{k+1}} = (-1)^k \frac{\left(\int_0^\beta d\tau |\vec{x}|^{2N} \right)^k}{k!} \tag{7.15}$$

thus we find

$$\frac{\operatorname{tr}\left(e^{-\beta H}\right)}{\operatorname{tr}\left(e^{-\beta H_0}\right)}\bigg|_k = \frac{(-1)^k}{k!}\mathcal{N}\int_{periodic}\mathcal{D}x(\tau)e^{-\left(\int_0^\beta d\tau\left(\frac{1}{2}\dot{\vec{x}}^2+\frac{1}{2}\vec{x}^2\right)-k\ln\left(\int_0^\beta d\tau|\vec{x}|^{2N}\right)\right)}. \quad (7.16)$$

To perform the path integral, we look for a critical point in $\vec{x}$, to the equation of motion

$$\ddot{\vec{x}} = \vec{x} - \frac{2Nk\vec{x}|\vec{x}|^{2(N-1)}}{\int_0^\beta d\tau|\vec{x}|^{2N}}. \quad (7.17)$$

Changing the scale by $\vec{x} \rightarrow \sqrt{\frac{2Nk}{\int_0^\beta d\tau|\vec{x}|^{2N}}}\vec{x}$ yields the equation

$$\ddot{\vec{x}} = \vec{x} - \vec{x}|\vec{x}|^{2(N-1)}. \quad (7.18)$$

The solution is easily found,

$$\vec{x} = \vec{u}x_0\left(\tau - \tau_0\right) \quad (7.19)$$

with $|\vec{u}|^2 = 1$ and the function x_0 given by,

$$(x_0\left(\tau\right))^{2(N-1)} = \frac{N}{\cosh^2\left((N-1)\tau\right)}, \quad (7.20)$$

where $x_0(\tau)$ satisfies

$$\ddot{x}_0 = x_0 - x_0(x_0)^{2(N-1)}. \quad (7.21)$$

This is most easily verified by observing

$$\frac{d}{d\tau}x_0^{2(N-1)} = \frac{-2N(N-1)\sinh(N-1)\tau}{\cosh^3(N-1)\tau} = -2x_0^{2(N-1)}(N-1)\tanh(N-1)\tau. \quad (7.22)$$

But

$$\frac{d}{d\tau}x_0^{2(N-1)} = 2(N-1)x_0^{2(N-1)-1}\dot{x}_0 \quad (7.23)$$

and therefore

$$\frac{d}{d\tau}x_0 = -x_0\tanh(N-1)\tau. \quad (7.24)$$

Finally

$$\begin{aligned}
\ddot{x}_0 &= -\dot{x}_0\tanh(N-1)\tau + x_0(N-1)\operatorname{sech}^2(N-1)\tau \\
&= x_0\tanh^2(N-1)\tau + x_0(N-1)\operatorname{sech}^2(N-1)\tau \\
&= x_0\left(1 - \operatorname{sech}^2(N-1)\tau - (N-1)\operatorname{sech}^2(N-1)\tau\right) \\
&= x_0\left(1 - \frac{N}{\cosh^2(N-1)\tau}\right) \\
&= x_0 - x_0(x_0)^{2(N-1)}
\end{aligned} \quad (7.25)$$

as required. Periodicity is satisfied if we begin at $\tau = \frac{\beta}{2}$ and end at $\tau = \frac{\beta}{2}$. As $\beta \rightarrow \infty$ the action is calculable,

$$S\left[\vec{u}x_0\left(\tau-\tau_0\right)\right] = Nk - Nk\ln\left(2Nk\right) + k(N-1)\ln(J), \quad (7.26)$$

where

$$J = \int_{-\infty}^{\infty} d\tau x_0^{2N}(\tau) = \frac{N^{\frac{N}{N-1}} 2^{\frac{N+1}{N-1}}}{N-1} \frac{\left(\Gamma\left(\frac{N}{N-1}\right)\right)^2}{\Gamma\left(\frac{2N}{N-1}\right)}. \tag{7.27}$$

It remains to calculate the determinant corresponding to the Gaussian fluctuations about this critical point. The operator coming from the second variation of the action is

$$\frac{\delta^2}{\delta x_\alpha(\tau_1)\delta x_\beta(\tau_2)} S(\vec{x})\Big|_{\vec{x}=\vec{u}x_0(\tau)} = \left(\left(-\frac{d^2}{d\tau_1^2} + 1 - \frac{N}{\cosh^2((N-1)\tau_1)}\right)\delta_{\alpha\beta}\right.$$
$$\left. - \frac{2(N-1)Nu_\alpha u_\beta}{\cosh^2((N-1)\tau_1)}\right)\delta(\tau_1-\tau_2)$$
$$+ \frac{2N}{J} u_\alpha u_\beta x_0^{2N-1}(\tau_1) x_0^{2N-1}(\tau_2)$$
$$= M_L u_\alpha u_\beta + M_T(\delta_{\alpha\beta} - u_\alpha u_\beta) \tag{7.28}$$

with

$$M_L = \left(-\frac{d^2}{d\tau_1^2} + 1 - \frac{(2N-1)N}{\cosh^2((N-1)\tau_1)}\right)\delta(\tau_1-\tau_2) + \frac{2N}{J} x_0^{2N-1}(\tau_1) x_0^{2N-1}(\tau_2) \tag{7.29}$$

and

$$M_T = \left(-\frac{d^2}{d\tau_1^2} + 1 - \frac{N}{\cosh^2((N-1)\tau_1)}\right)\delta(\tau_1-\tau_2). \tag{7.30}$$

For the transverse operator M_T, the corresponding "quantum mechanical" Hamiltonian is

$$H = p^2 - \frac{\lambda(\lambda+1)}{\cosh^2(x)}, \tag{7.31}$$

which is exactly solvable. The eigenfunctions are the Jacobi functions. The ratio of the determinants is given by

$$\frac{\det(H-z)}{\det(H_0-z)} = \frac{\Gamma\left(1+\sqrt{-z}\right)\Gamma\left(\sqrt{-z}\right)}{\Gamma\left(1+\lambda+\sqrt{-z}\right)\Gamma\left(\sqrt{-z}-\lambda\right)}, \tag{7.32}$$

which is calculated using the Affleck Coleman method [31, 114, 36], where Γ is the usual gamma function. For the case at hand, $\lambda = \frac{1}{N-1}$, $z = -\frac{1}{(N-1)^2}$ which gives the transverse operator up to a factor of $1/(N-1)^2$. We must separate out the zero modes. These arise because of the invariance of the original Hamiltonian under global rotations of $\vec{x}$ (equivalently of $\vec{u}$). Rotations about a direction orthogonal to $\vec{u}$ should all be in the transverse operator. Thus the zero mode for M_T is simply $x_0(\tau)$.

$$\delta_{rot.}(\vec{u}x_0(\tau)) = (\delta\vec{u})x_0(\tau), \tag{7.33}$$

where $(\delta \vec{u})$ counts the number of independent rotations. To find $\frac{\det'(H-z)}{\det(H_0-z)}$, we must divide the ratio by the smallest eigenvalue for λ not equal to its critical value, and then take the limit. Now

$$H - z = -\frac{d^2}{dx^2} - \frac{\lambda(\lambda+1)}{\cosh^2(x)} - z; \qquad (7.34)$$

however, if we scale $x \to (N-1)t$, with $\lambda = \frac{1}{N-1}$, $z = -\frac{1}{(N-1)^2}$, we get

$$H - z = \frac{1}{(N-1)^2}\left(-\frac{d^2}{dt^2} - \frac{N}{\cosh^2((N-1)t)} + 1\right). \qquad (7.35)$$

Then with $z = -\frac{1}{(N-1)^2} + \epsilon$ the zero mode becomes an eigenmode with eigenvalue ϵ. Each eigenvalue of $H - z$ is $\frac{1}{(N-1)^2}$ times the eigenvalue of $-\frac{d^2}{dt^2} - \frac{N}{\cosh^2((N-1)t)} + 1$. Thus we must divide by $\epsilon(N-1)^2$ to get det$'$. Hence

$$\lim_{z \to -\frac{1}{(N-1)^2}} \frac{2\pi}{\left(-\frac{1}{(N-1)^2} - z\right)(N-1)^2} \frac{\det(H-z)}{\det(H_0-z)} = \frac{2\pi(N+1)}{2(N-1)} \frac{\Gamma^2\left(\frac{N}{N-1}\right)}{\Gamma\left(\frac{2N}{N-1}\right)} \quad (7.36)$$

The 2π comes from the definition of the measure in the Gaussian integral. There are $n-1$-independent transverse directions, for each one we have the same det$'$, to the power $-\frac{1}{2}$, giving the total power $-\frac{n-1}{2}$. The Jacobian factor coming from changing the integration variable from the zero mode "Gaussian fluctuation" to the integration over the position gives a factor of $\sqrt{\int_{-\infty}^{\infty} d\tau x_0^2(\tau)} = (k(N+1))^{\frac{1}{2}}$. Thus the total contribution of the transverse modes is

$$\frac{(2\pi)^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}\right)}(k(N+1))^{\frac{n-1}{2}} \left[\frac{\pi(N+1)}{(N-1)} \frac{\Gamma^2\left(\frac{N}{N-1}\right)}{\Gamma\left(\frac{2N}{N-1}\right)}\right]^{-\frac{n-1}{2}}. \qquad (7.37)$$

The first factor is the volume from integrating over the directions of $\vec{u}$. The longitudinal operator can also be treated in a similar fashion. With

$$M_L = \bar{M}_L + |u\rangle\langle u|$$
$$\bar{M}_L = -\frac{d^2}{dt^2} + 1 - \frac{(2N-1)N}{\cosh^2((N-1)t)} \qquad (7.38)$$

where $|u\rangle\langle u|$ projects on the mode $x_0^{2N-1}(\tau)$. There is one zero mode coming from time translation invariance, $\frac{dx_0(\tau)}{d\tau}$. It is orthogonal to $x_0^{2N-1}(\tau)$

$$\int_{-\infty}^{\infty} d\tau x_0^{2N-1}(\tau) \frac{dx_0(\tau)}{d\tau} = \int_{-\infty}^{\infty} d\tau \frac{d}{d\tau} \frac{x_0^{2N}(\tau)}{2N} = \left.\frac{x_0^{2N}(\tau)}{2N}\right|_{-\infty}^{\infty} = 0 \qquad (7.39)$$

Then with $|v\rangle$ denoting eigenstates orthogonal to $|u\rangle$

$$
\begin{aligned}
\det\left(\bar{M}_L + |u\rangle\langle u|\right) &= \det\left(\bar{M}_L\right)\det\left(1 + \bar{M}_L^{-1}|u\rangle\langle u|\right) \\
&= \det\left(\bar{M}_L\right)\det\left(1 + \left(|u\rangle\langle u| + \sum_v |v\rangle\langle v|\right)\bar{M}_L^{-1}|u\rangle\langle u|\right) \\
&= \det\left(\bar{M}_L\right)\det\left(1 + \langle u|\bar{M}_L^{-1}|u\rangle|u\rangle\langle u| + \sum_v \langle v|\bar{M}_L^{-1}|u\rangle|v\rangle\langle u|\right) \\
&= \det\left(\bar{M}_L\right)\left(1 + \langle u|\bar{M}_L^{-1}|u\rangle\right)
\end{aligned}
\tag{7.40}
$$

where the final equality follows because the second determinant is of a matrix that is upper triangular. From the equation of motion

$$
\frac{\bar{M}_L}{2(1-N)}x_0 = x_0^{2N-1}.
\tag{7.41}
$$

Thus

$$
\begin{aligned}
\langle u|\bar{M}_L^{-1}|u\rangle &= \frac{\int_{-\infty}^{\infty} d\tau\, x_0^{2N-1}\bar{M}_L^{-1}x_0^{2N-1}}{\int_{-\infty}^{\infty} d\tau\,\left(x_0^{2N-1}\right)^2} \\
&= \frac{1}{2(1-N)}\frac{\int_{-\infty}^{\infty} d\tau\, x_0^{2N-1}x_0}{\int_{-\infty}^{\infty} d\tau\,\left(x_0^{2N-1}\right)^2}.
\end{aligned}
\tag{7.42}
$$

The integrals can be done exactly, giving

$$
\det\left(M_L\right) = \frac{-1}{(N-1)}\det\left(\bar{M}_L\right)
\tag{7.43}
$$

$\bar{M}_L$ has a negative mode, which cancels the minus sign. This is not an instability, $\bar{M}_L$ is just an auxilliary operator. Now we have an operator of the same form as the transverse part before

$$
H - z = -\frac{d^2}{dx^2} + \frac{\lambda(\lambda+1)}{\cosh^2(x)} - z
\tag{7.44}
$$

with $\lambda = \frac{N}{N-1}$, and $z = \frac{-1}{(N-1)^2}$. Then the $\det'$ is,

$$
\lim_{z\to\frac{-1}{(N-1)^2}}\left.\frac{\det'(H-z)}{\det(H_0-z)}\right|_{\lambda=\frac{N}{N-1}} = -2\pi\frac{1}{2}\frac{\Gamma^2\left(\frac{N}{N-1}\right)}{\Gamma\left(\frac{2N}{N-1}\right)}
\tag{7.45}
$$

The Jacobian from the usual change of variables in the integration is

$$
\left(\int_{-\infty}^{\infty} d\tau\left(\frac{dx_0}{d\tau}\right)^2\right)^{\frac{1}{2}} = (k(N-1))^{\frac{1}{2}},
\tag{7.46}
$$

which then gives the total contribution

$$
\beta\left(\frac{1}{N-1}2\pi\frac{1}{2}\frac{\Gamma^2\left(\frac{N}{N-1}\right)}{\Gamma\left(\frac{2N}{N-1}\right)}\right)^{-\frac{1}{2}}(k(N-1))^{\frac{1}{2}},
\tag{7.47}
$$

where the β comes from the integration over the position of the instanton. Finally, putting all the pieces together, we get the correction to the kth order in perturbation to the energy splitting

$$\mathcal{E} - \mathcal{E}_0 = (-1)^{k+1} g^k \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \frac{((N-1))^{\frac{n+1}{2}} k^{\frac{n-1}{2}}}{\Gamma\left(\frac{n}{2}\right) 2^k} \left(\frac{\Gamma\left(\frac{2N}{N-1}\right)}{\Gamma^2\left(\frac{N}{N-1}\right)}\right)^{k(N-1)+\frac{n}{2}}$$

$$\times e^{k(N-1)\ln\left(\frac{k(N-1)}{e}\right)} \left(1 + o(g)\right). \tag{7.48}$$

7.3 Generalization to Field Theory

This result can be generalized to the case of quantum field theory; we leave this for the reader. We should make one point, though. Generally, we do not believe that the functional integral is an analytic function in an annulus around the point $g = 0$ in the g-plane. Indeed, for g negative the Hamiltonian is not self-adjoint for sufficiently large N. We expect that in reality $\mathcal{I}(g)$ is defined in the complex plane by analytic continuation, and this analytic function has a branch cut along the negative real axis which terminates at $g = 0$. We must use the once subtracted dispersion relation

$$\mathcal{I}(g) = -\frac{1}{2\pi i} \int_0^R d\lambda \frac{1}{\lambda + g} \left(\mathcal{I}(-\lambda + i\epsilon) - \mathcal{I}(-\lambda - i\epsilon)\right) + \frac{1}{2\pi i} \int_{|g'|=R} \frac{\mathcal{I}(g)}{(g' - g)}, \tag{7.49}$$

which corresponds to the contour in Figure 7.1. If the second integral vanishes as $R \to \infty$ we get

$$\mathcal{I}(g) = -\frac{1}{2\pi i} \int_0^\infty d\lambda \frac{1}{\lambda + g} \left(\text{discontinuity}\left(\mathcal{I}(-\lambda)\right)\right). \tag{7.50}$$

For

$$\mathcal{I}(g) = \sum_k \mathcal{I}_k g^k \tag{7.51}$$

we have

$$\mathcal{I}_k = -(-1)^k \frac{1}{2\pi i} \int_0^\infty d\lambda \frac{1}{\lambda^{k+1}} \left(\text{discontinuity}\left(\mathcal{I}(-\lambda)\right)\right). \tag{7.52}$$

The factor $1/\lambda^{k+1}$ becomes more and more singular at the end point $\lambda = 0$; thus, if we know how the discontinuity of $\mathcal{I}(-\lambda)$ behaves for small λ, we can find the behaviour of $\mathcal{I}_k$ for large k. For an expected asymptotic behaviour

$$\text{discontinuity}\left(\mathcal{I}(-\lambda)\right) \sim 2iBe^{-\frac{S_c}{\lambda}} \lambda^{-\alpha} \sum_l a_l \lambda^l \tag{7.53}$$

implies directly

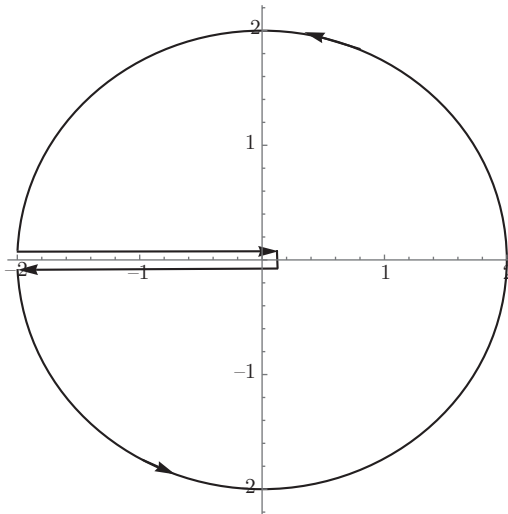$$\mathcal{I}_k \sim -\frac{1}{\pi}(-1)^k B \sum_l a_l \Gamma(k + \alpha - l) S_c^{-(k+\alpha-l)}. \tag{7.54}$$

Figure 7.1. Integration contour in the complex g plane for field theory

The discontinuity of discontinuity $(\mathcal{I}(-\lambda))$ can actually be computed using the semi-classical methods that we have been learning about. Collins and Soper [35] show that it has an expansion of exactly the form given in Equation (7.53). Thus the formal calculations that we have done, not worrying about the cut in the complex g plane, produce the same results with much less difficulty.

7.4 Instantons and Quantum Spin Tunnelling

We continue this chapter with an application to quantum spin tunnelling. This calculation starts out as an independent tunnelling calculation that, in principle, has nothing to do with large orders in perturbation theory. However, it turns out that the tunnelling calculations are all attainable through large orders in perturbation theory. We will have to understand what spin-coherent states are and the corresponding path integral.

7.5 Spin-Coherent States and the Path Integral for Spin Systems

For a spin system, instead of the orthogonal position $|x\rangle$ and momentum $|p\rangle$ basis we define a basis of spin-coherent states [106, 100, 75, 87]. Let $|s, s\rangle$ be the highest weight vector in a particular representation of the rotation group. This state is taken to be an eigenstate of the operators $\hat{S}_z$ and $\hat{S}$, two mutually commuting operators:

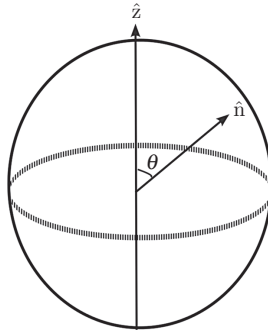$$\hat{S}_z |s,s\rangle = s |s,s\rangle \quad \hat{S}^2 |s,s\rangle = s(s+1)|s,s\rangle. \tag{7.55}$$

Figure 7.2. The directions of the unit vectors $\hat{z}$ and $\hat{n}$ on a two-sphere

The spin operators $\hat{S}_i$, $i = x, y, z$ satisfy the Lie algebra of $SU(2)$,

$$[\hat{S}_i, \hat{S}_j] = i\epsilon_{ijk}\hat{S}_k \tag{7.56}$$

where ϵ_{ijk} is the totally antisymmetric tensor symbol and summation over repeated indices is implied in Equation (7.56).

The coherent state is defined as [100, 87, 75, 127, 49, 48]

$$|\hat{n}\rangle = e^{i\theta\hat{m}\cdot\hat{S}}|s, s\rangle = \sum_{m=-s}^{s} \mathcal{M}^s(\hat{n})_{ms}|s, m\rangle, \tag{7.57}$$

where $|\hat{n}\rangle$ is an element of the $2s + 1$-dimensional Hilbert (representation) space for the spin states, $\hat{n} = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)$ is a unit vector, *i.e.* $\hat{n}^2 = 1$ and $\hat{m} = (\hat{n} \times \hat{z})/|\hat{n} \times \hat{z}|$ is a unit vector orthogonal to $\hat{n}$ and $\hat{z}$. $\hat{z}$ is the quantization axis pointing from the origin to the north pole of a unit sphere and $\hat{n} \cdot \hat{z} = \cos\theta$ as shown in Figure 7.2. Rotating the unit vector $\hat{n}$ counterclockwise about the $\hat{m}$ direction by the angle θ brings it exactly to the unit vector $\hat{z}$. $|\hat{n}\rangle$ corresponds to a rotation of an eigenstate of $\hat{S}_z$, i.e $|s, s\rangle$, to an eigenstate with a quantization axis along $\hat{n}$ on a two-dimensional sphere $\mathcal{S}^2 = SU(2)/U(1)$. It turns out that the matrices $\mathcal{M}^s(\hat{n})$ satisfy a non-trivial relation

$$\mathcal{M}^s(\hat{n}_1)\mathcal{M}^s(\hat{n}_2) = \mathcal{M}^s(\hat{n}_3)e^{i\mathcal{G}(\hat{n}_1, \hat{n}_2, \hat{n}_3)\hat{S}_z} \tag{7.58}$$

where $\mathcal{G}(\hat{n}_1, \hat{n}_2, \hat{n}_3)$ is the area of a spherical triangle with vertices $\hat{n}_1, \hat{n}_2, \hat{n}_3$. Note that Equation (7.58) is not a group multiplication, thus the matrices $\mathcal{M}^s(\hat{n})$ do not form a group representation and $\mathcal{G}(\hat{n}_1, \hat{n}_2, \hat{n}_3)$ is called a co-cycle, which represents the obstruction that the matrices $\mathcal{M}^s(\hat{n})$ exhibit to forming a true representation of the rotation group.

Unlike normal position and momentum eigenstates, the inner product of two coherent states is not orthogonal:

$$\langle\hat{n}|\hat{n}'\rangle = e^{is\mathcal{G}(\hat{n}, \hat{n}', \hat{z})}[\frac{1}{2}(1 + \hat{n} \cdot \hat{n}')]^s \tag{7.59}$$

It has the following property:

$$\hat{n} \cdot \hat{S} |\hat{n}\rangle = s |\hat{n}\rangle \Rightarrow \langle \hat{n}|\hat{S}|\hat{n}\rangle = s\hat{n} \tag{7.60}$$

while the resolution of identity is given by

$$\hat{I} = \frac{2s+1}{4\pi} \int d^3\hat{n}\,\delta(\hat{n}^2 - 1) |\hat{n}\rangle \langle \hat{n}|, \tag{7.61}$$

where $\hat{I}$ is a $(2s+1) \times (2s+1)$ identity matrix, and the delta function ensures that $\hat{n}^2 = 1$. Using the expression in Equations (7.59) and (7.61) we can express the imaginary time transition amplitude between $|\hat{n}_i\rangle$ and $|\hat{n}_f\rangle$ as a path integral, which for the spin system is given by [48, 127]

$$\langle \hat{n}_f| e^{-\beta \hat{H}(\hat{S})}|\hat{n}_i\rangle = \int \mathcal{D}\hat{n}\, e^{-S_E[\hat{n}]}, \tag{7.62}$$

where

$$S_E[\hat{n}] = is S_{WZ} + \int d\tau U(\hat{n}(\tau)), \quad U(\hat{n}(\tau)) = \langle \hat{n}|\hat{H}|\hat{n}\rangle \tag{7.63}$$

and S_{WZ} arises because of the additional phase $e^{is\mathcal{G}(\hat{n},\hat{n}',\hat{z})}$ in Equation (7.59). We have set $\hbar = 1$ in the path integral.

The Wess–Zumino (WZ) action, S_{WZ} in the coordinate independent formalism, is given by[1] [97, 122, 120, 49, 48]

$$S_{WZ} = \int_{\frac{1}{2}\mathcal{S}^2} d\tau d\xi\, \hat{n}(\tau,\xi) \cdot [\partial_\tau \hat{n}(\tau,\xi) \times \partial_\xi \hat{n}(\tau,\xi)], \tag{7.64}$$

where $\hat{n}(\tau)$ has been extended over a topological half-sphere $\frac{1}{2}\mathcal{S}^2$ in the variables τ, ξ. We call this the coordinate independent expression since no system of coordinates is specified for the unit vector $\hat{n}$. In the topological half-sphere we define $\hat{n}$ with the boundary conditions

$$\hat{n}(\tau,0) = \hat{n}(\tau), \ \hat{n}(\tau,1) = \hat{z} \tag{7.65}$$

so that the original configuration lies at the equator and the point $\xi = 1$ is topologically compactified by the boundary condition. This can be easily obtained by imagining that the original closed loop $\hat{n}(\tau)$ at $\xi = 0$ is simply pushed up along the meridians to $\hat{n}(\tau) = \hat{z}$ at $\xi = 1$. The WZ term originates from the non-orthogonality of spin-coherent states in Equation (7.59). Geometrically, it defines the area of the closed loop on the spin space, defined by the nominally periodic, original configuration $\hat{n}(\tau)$. It is crucial to note that there is an ambiguity of modulo 4π, since different ways of pushing the original configuration up to the north pole can give different values for the area enclosed by the closed loop as we can imagine that the closed loop englobes the whole two sphere any integer number of times, but this ambiguity has no physical significance since

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[1] An alternative way of deriving this equation can be found in [16].

$e^{iN4\pi s} = 1$ for integer and half-odd integer s. The action, Equation (7.63), is valid for a semi-classical spin system whose phase space is $\mathcal{S}^2$. It is the starting point for studying macroscopic quantum spin tunnelling between the minima of the energy $U(\hat{n})$.

7.6 Coordinate-Independent Formalism

In the coordinate independent formalism, the spin is represented by a unit vector $\hat{n}(\tau)$ but no parametrization of the unit vector is assumed. It is best to exemplify the coordinate independent analysis through an explicit system.

We will study the simplest biaxial single-molecule magnet whose spin Hamiltonian is given by

$$H = -K_z \hat{S}_z^2 + K_y \hat{S}_y^2, \quad K_z \gg K_y > 0. \tag{7.66}$$

The above Hamiltonian possesses an easy-axis in the z-direction and a hard-axis in the y-direction. When $K_y = 0$, the spin is localized along the z-axis, which is usually parameterized by the variable $\theta = 0, \pi$ and possesses two degenerate minima localized at the north and the south poles of the two-sphere of phase space. Addition of small $K_y \neq 0$ introduces dynamics into the system and causes tunnelling. The real tunnelling variable is expected to be θ in the easy-axis direction.

The Hamiltonian defined above has been studied in the presence of a magnetic field by many authors [28, 27, 53]. However, the quantum-phase interference for this model has not been computed, due to the subtlety involved in computing the action for the instanton. Since the relation $\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2 = s(s+1)$ holds for any spin system, it is evident that any biaxial single-molecule magnet is related to any other either by rescaling the anisotropy constant or by rotation of axes. For instance, the Hamiltonian studied by Enz and Schilling [43]:

$$H = -A\hat{S}_x^2 + B\hat{S}_z^2, \quad (h = 0), \tag{7.67}$$

possesses an easy x-axis and a hard z-axis. This model in the conventional spherical parametrization in terms of the phase space variables, $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is exactly our Hamiltonian Equation (2.15) in the unconventional spherical parametrization $\hat{n} = (\sin\theta\sin\phi, \cos\theta, \sin\theta\cos\phi)$ with $K_z = A$ and $K_y = B$.

7.6.1 Coordinate-Dependent Analysis

To demonstrate the technique for investigating the quantum-phase interference in the z-easy-axis model, we will first keep to the conventional, coordinate-dependent spherical parametrization, $\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. It was shown [52] that perturbation theory in the K_y term for integer spin leads

to an energy-splitting proportional to $(K_y)^s$ while for half-odd integer spin, the splitting vanishes in accordance with Kramers' theorem. We will recover this result using the spin-coherent state path integral, and we will explicitly demonstrate in all detail that the result can be obtained without recourse to a coordinate-dependent parametrization.

The transition amplitude in the spin-coherent state path integral, in the coordinate-dependent formalism, is given by [75]

$$\langle \theta_f, \phi_f | e^{-\beta H} | \theta_i, \phi_i \rangle = \int \mathcal{D}[\cos\theta] \mathcal{D}[\phi] e^{-S_E/\hbar} \qquad (7.68)$$

where the Euclidean action is

$$S_E = \int d\tau \left[is\dot\phi(1 - \cos\theta) + E(\theta, \phi) \right] \qquad (7.69)$$

where the first term is the WZ term in the coordinate dependent formalism and the classical anisotropy energy Equation (2.15) is

$$E(\theta, \phi) = (K_z + K_y \sin^2\phi)\sin^2\theta. \qquad (7.70)$$

We note that the WZ term, being first-order in time derivatives, remains imaginary upon analytic continuation to Euclidean time. This has important ramifications for the putative instanton solutions: they too must have non-trivial imaginary parts. The classical degenerate ground states correspond to $\phi = 0$, $\theta = 0, \pi$, that is the spin is pointing in the north or south pole of the two-sphere. The classical equations of motion obtained by varying the action with respect to θ and ϕ, respectively, are

$$is\dot\phi\sin\theta = -\frac{\partial E(\theta, \phi)}{\partial\theta} \qquad (7.71)$$

$$is\dot\theta\sin\theta = \frac{\partial E(\theta, \phi)}{\partial\phi}. \qquad (7.72)$$

It is evident from these two equations, because of the explicit i, that one variable has to be imaginary for the equations to be consistent. The only appropriate choice is to take real θ and imaginary ϕ, since the real tunnelling coordinate (z-easy-axis) is θ. This comes out naturally from the conservation of energy, which follows by multiplying Equation (7.72) by $\dot\phi$ and Equation (7.71) by $\dot\theta$ and subtracting the two:

$$\frac{dE(\theta, \phi)}{d\tau} = 0 \quad \text{i.e,} \quad E(\theta, \phi) = \text{const.} = 0, \qquad (7.73)$$

the normalization coming from the value at $\theta = 0$. Thus,

$$E(\theta, \phi) = (K_z + K_y \sin^2\phi)\sin^2\theta = 0. \qquad (7.74)$$

Since $\sin^2\theta \neq 0$, as it must vary from 0 to π, it follows that,

$$\sin\phi = \pm i\sqrt{\frac{K_z}{K_y}}, \qquad (7.75)$$

therefore ϕ is imaginary and constant. Let $\phi = \phi_R + i\phi_I$, then $\sin\phi = \sin\phi_R\cosh\phi_I + i\cos\phi_R\sinh\phi_I$. We must take $\phi_R = n\pi$ so that $\sin\phi_R = 0$ as the right-hand side of Equation (7.75) is imaginary. Hence

$$(-1)^n \sinh\phi_I = \pm\sqrt{\frac{K_z}{K_y}}, \tag{7.76}$$

as $\cos\phi_R = (-1)^n$. There are four solutions of this equation: $n = 0$, $\phi = i\phi_I$ and $n = 1$, $\phi = \pi - i\phi_I$ for the positive sign and $n = 0$, $\phi = -i\phi_I$ and $n = 1$, $\phi = \pi + i\phi_I$ for the negative sign, where ϕ_I is the same in both cases. Taking into account that $K_z \gg K_y > 0$, we have $\phi_I = \text{arcsinh}\left(\sqrt{\frac{K_z}{K_y}}\right) \approx \frac{1}{2}\ln\left(\frac{4K_z}{K_y}\right)$.

The classical equation of motion (7.72) simplifies to

$$is\frac{\dot{\theta}}{\sin\theta} = K_y \sin 2\phi = iK_y \sinh 2\phi_I \tag{7.77}$$

The solution is easily found as

$$\theta(\tau) = 2\arctan[\exp(\omega(\tau - \tau_0))], \tag{7.78}$$

where $\omega = \frac{K_y}{s}\sinh 2\phi_I$. This corresponds to the tunnelling of the state $|\uparrow\rangle$ from $\theta(\tau) = 0$ at $\tau = -\infty$ to the state $|\downarrow\rangle$, $\theta(\tau) = \pi$ at $\tau = \infty$. The two solutions $\phi = i\phi_I$ and $\phi = \pi + i\phi_I$ in the upper-half plane of complex ϕ correspond to the instanton, ($\dot{\theta} > 0$) while the solutions $\phi = -i\phi_I$ and $\phi = \pi - i\phi_I$ in the lower-half plane of complex ϕ correspond to the anti-instanton, ($\dot{\theta} < 0$).

Since the energy, $E(\theta, \phi)$, in the action Equation (7.69) is conserved and therefore always remains zero along this trajectory, the action for this path is determined only by the WZ term which is given by

$$S_E = S_{WZ} = is\int_{-\infty}^{\infty} d\tau\,\dot{\phi}(1 - \cos\theta) = is\int_{\phi_i}^{\phi_f} d\phi(1 - \cos\theta). \tag{7.79}$$

Naively, one can use the fact that ϕ is constant and hence $\dot{\phi} = 0$, which seems to give $S_{WZ} = 0$; however, care must be taken when computing the action. A non-zero Euclidean action is found by realizing, as in [99], that we must take into account the fact that ϕ must be translated from $\phi = 0$ to $\phi = n\pi + i\phi_I$ before the instanton can occur and then back to $\phi = 0$ after the instanton has occurred. Since the action is linear in time derivative of ϕ, the actual path taken does not matter, only the boundary values matter. In the present problem, we have two solutions for ϕ, *i.e.* $\phi = i\phi_I$ and $\phi = \pi + i\phi_I$ corresponding to two instanton paths, call them I and II. The full action is then

$$S_E^I = is\int_0^{\pi + i\phi_I} d\phi(1 - \cos\theta)|_{\theta=0} + is\int_{\pi + i\phi_I}^0 d\phi(1 - \cos\theta)|_{\theta=\pi}$$
$$= -2\pi is + 2s\phi_I \tag{7.80}$$

and

$$S_E^{II} = is \int_0^{i\phi_I} d\phi(1 - \cos\theta)|_{\theta=0} \tag{7.81}$$

$$+ is \int_{i\phi_I}^0 d\phi(1 - \cos\theta)|_{\theta=\pi} = 2s\phi_I,$$

where it is clear that the total derivative term $d\phi$ contributes nothing as the two contributions cancel in the round trip, while the $d\phi \cos\theta$ gives all the answer, since $\cos\theta = 1$ initially, before the instanton has occurred, while $\cos\theta = -1$ after. The action for the corresponding anti-instantons is identical. The amplitude for the transition from $\theta = 0$ to $\theta = \pi$, as usual, is calculated by summing over a sequence of one instanton followed by an anti-instanton with an odd total number of instantons and anti-instantons [31], but we must add the two exponentials of the actions S_E^I and S_E^{II} for both instanton and anti-instanton. We note

$$e^{S_E^I} + e^{S_E^{II}} = e^{-2s\phi_I}\left(1 + e^{2\pi is}\right) = e^{-2s\phi_I}\left(1 + \cos 2\pi s\right), \tag{7.82}$$

where the last factor vanishes for half-odd integer spin. Then we get that the expression for the amplitude is given by

$$\langle \pi | e^{-\beta\hat{H}} | 0 \rangle = \mathcal{N} \sinh\left(\kappa\beta(1 + \cos(2\pi s))e^{-2s\phi_I}\right) \tag{7.83}$$

where κ is the properly normalized square root of the determinant of the operator governing the second-order fluctuations without the zero mode, which we have not computed, and $\mathcal{N}$ is the usual normalization factor. The energy splitting can be read off from this expression

$$\Delta E = \kappa(1 + \cos(2\pi s))e^{-2s\phi_I}. \tag{7.84}$$

For half-odd integer spin the splitting vanishes, while for integer spin we have

$$\Delta E = 4\kappa \left(\frac{K_y}{4K_z}\right)^s \tag{7.85}$$

which agrees with the result found by perturbation theory [52].

7.6.2 Coordinate-Independent Analysis

Now we wish to see that the spherical-polar coordinate-dependent parametrization of the unit vector $\hat{n}$ is not at all necessary. Then the action for the Hamiltonian in Equation (7.66) can be written as

$$S_E = \int d\tau \mathcal{L}_E = \int d\tau \left[-K_z(\hat{n}\cdot\hat{z})^2 + K_y(\hat{n}\cdot\hat{y})^2\right]$$

$$+ is \int d\tau d\xi \left[\hat{n}\cdot(\partial_\tau\hat{n}\times\partial_\xi\hat{n})\right]. \tag{7.86}$$

The first term is the anisotropy energy while the second term is the WZ term written in a coordinate-independent form. The WZ term is integrated over a two manifold whose boundary is physical, Euclidean time τ. Thus the configuration in τ is extended into a second dimension with coordinate ξ. The equations of motion arise from variation with respect to $\hat{n}$. However, $\hat{n}$ is a unit vector, hence its variation is not arbitrary, indeed, $\hat{n} \cdot \delta\hat{n} = 0$. Thus, to obtain the equations of motion, we vary $\hat{n}$ as if it is not constrained, but then we must project on to the transverse part of the variation:

$$\delta_{\hat{n}} S_E = 0 \Rightarrow \int d\tau (\delta_{\hat{n}} \mathcal{L}_E) \cdot \delta\hat{n} = 0 \Rightarrow \hat{n} \times (\delta_{\hat{n}} \mathcal{L}_E) = 0. \qquad (7.87)$$

Taking the cross-product of the resulting equation one more time with $\hat{n}$ does no harm, and this process yields the equations of motion

$$is\partial_\tau \hat{n} - 2K_z (\hat{n} \cdot \hat{z})(\hat{n} \times \hat{z}) + 2K_y (\hat{n} \cdot \hat{y})(\hat{n} \times \hat{y}) = 0. \qquad (7.88)$$

Taking the cross-product of this equation with $\partial_\tau \hat{n}$, the first term vanishes as the vectors are parallel, yielding

$$-2K_z (\hat{n} \cdot \hat{z})\partial_\tau \hat{n} \times (\hat{n} \times \hat{z}) + 2K_y (\hat{n} \cdot \hat{y})\partial_\tau \hat{n} \times (\hat{n} \times \hat{y}) = 0. \qquad (7.89)$$

Simplifying the triple vector product, using $\partial_\tau \hat{n} \cdot \hat{n} = 0$, and then taking the scalar product of the subsequent equation with $\hat{n}$ gives

$$\partial_\tau \left(-K_z (\hat{n} \cdot \hat{z})^2 + K_y (\hat{n} \cdot \hat{y})^2 \right) = 0, \qquad (7.90)$$

which is the conservation of energy. The initial value of $\hat{n} = \hat{z}$ says that the energy must equal

$$\left(-K_z (\hat{n} \cdot \hat{z})^2 + K_y (\hat{n} \cdot \hat{y})^2 \right) = -K_z. \qquad (7.91)$$

From this equation and because $\hat{n}$ is a unit vector we find

$$\hat{n} \cdot \hat{y} = \pm \sqrt{\frac{K_z}{K_y} ((\hat{n} \cdot \hat{z})^2 - 1)} = \pm i \sqrt{\frac{K_z}{K_y} (1 - (\hat{n} \cdot \hat{z})^2)}$$

$$\hat{n} \cdot \hat{x} = \pm \sqrt{\frac{K_y + K_z}{K_y} (1 - (\hat{n} \cdot \hat{z})^2)}, \qquad (7.92)$$

where the $\pm$ signs are not correlated. Then

$$\frac{\hat{n} \cdot \hat{y}}{\hat{n} \cdot \hat{x}} = \pm i \sqrt{\frac{K_z}{K_y + K_z}} = \tan\phi; \qquad (7.93)$$

hence, we recover the result immediately that ϕ is a complex constant, just as before. Taking the scalar product of Equation (7.88) with $\hat{z}$ yields

$$is\partial_\tau (\hat{n} \cdot \hat{z}) + 2K_y (\hat{n} \cdot \hat{y})(\hat{n} \cdot \hat{x}) = 0 \qquad (7.94)$$

and replacing from Equation (7.92) gives

$$is\partial_\tau(\hat{n}\cdot\hat{z}) \pm 2i\sqrt{K_z(K_y+K_z)}(1-(\hat{n}\cdot\hat{z})^2) = 0 \tag{7.95}$$

Notice that the i's neatly cancel leaving a trivial, real differential equation for $\hat{n}\cdot\hat{z}$, which we can write as

$$\frac{\partial_\tau(\hat{n}\cdot\hat{z})}{1-(\hat{n}\cdot\hat{z})} + \frac{\partial_\tau(\hat{n}\cdot\hat{z})}{1+(\hat{n}\cdot\hat{z})} = \pm\frac{4}{s}\sqrt{K_z(K_y+K_z)}. \tag{7.96}$$

This integrates as

$$\ln\frac{1+(\hat{n}\cdot\hat{z})}{1-(\hat{n}\cdot\hat{z})} = \pm\frac{4}{s}\sqrt{K_z(K_y+K_z)}(\tau-\tau_0). \tag{7.97}$$

Exponentiating and solving for $\hat{n}\cdot\hat{z}$ gives

$$\hat{n}\cdot\hat{z} = \pm\tanh\left(\frac{2}{s}\sqrt{K_z(K_y+K_z)}(\tau-\tau_0)\right), \tag{7.98}$$

which is exactly the same as the solution found for θ in Equation (7.78). The instanton (upper sign) interpolates from $n_z = 1$ to $n_z = -1$ as $\tau \to \pm\infty$.

Thus it is important to know that the equations of motion can be solved without recourse to a specific choice for the coordinates. We will now evaluate the tunnelling amplitude and the quantum interference directly in terms of the coordinate-independent variables. Since the energy remains constant along the instanton trajectory, the action is determined entirely from the WZ term

$$S_{WZ} = is\int d\tau \int_0^1 d\xi\left[\hat{n}\cdot(\partial_\tau\hat{n}\times\partial_\xi\hat{n})\right]. \tag{7.99}$$

The integration over ξ can be done explicitly by writing the unit vector as

$$\hat{n}(\tau,\xi) = f(\tau,\xi)n_z(\tau)\hat{z} + g(\tau,\xi)[n_x(\tau)\hat{x} + n_y(\tau)\hat{y}] \tag{7.100}$$

with the boundary conditions $\hat{n}(\tau,\xi=0) = \hat{n}(\tau)$ and $\hat{n}(\tau,\xi=1) = \hat{z}$, where we write n_z for $\hat{n}(\tau)\cdot\hat{z}$, etc. Using the expression in Equations (7.100) and the condition that $\hat{n}\cdot\hat{n} = 1$, one obtains

$$g^2 = \frac{1-f^2n_z^2}{1-n_z^2} \tag{7.101}$$

These functions obey the boundary conditions

$$f(\tau,\xi=0) = 1, f(\tau,\xi=1) = \frac{1}{n_z(\tau)},$$
$$g(\tau,\xi=0) = 1, g(\tau,\xi=1) = 0 \tag{7.102}$$

The integrand of Equation (7.99) can now be written in terms of the functions defined in Equation (7.100). After a straightforward, but rather tedious,

calculation we obtain

$$\hat{n} \cdot (\partial_\tau \hat{n} \times \partial_\xi \hat{n}) = n_z (g^2 f' - fg g')(n_x \dot{n}_y - n_y \dot{n}_x)$$

$$= \frac{n_z f'}{1 - n_z^2}(n_x \dot{n}_y - n_y \dot{n}_x), \tag{7.103}$$

where $f' \equiv \partial_\xi f$, $\dot{n}_{x,y} \equiv \partial_\tau n_{x,y}$. The second equality follows from Equation (7.101). Replacing Equation (7.103) into the WZ term, the ξ integration in Equation (7.99) can be done explicitly which yields

$$S_{WZ} = is \int d\tau \frac{(n_x \dot{n}_y - n_y \dot{n}_x)}{1 + n_z}. \tag{7.104}$$

This expression defines the WZ term in the coordinate-independent form as a function of time alone. We can always make recourse to any specific coordinates, taking the z-easy-axis system, with the spherical parameterization we recover the usual form of the WZ term in condensed matter physics, *i.e.* Equation (7.79). Multiplying the top and the bottom of the integrand in Equation (7.104) by $(1 - n_z)$, the resulting integrand simplifies to

$$S_{WZ} = is \int \frac{d(n_y/n_x)}{1 + (n_y/n_x)^2}(1 - n_z)$$

$$= is \int d[\arctan(n_y/n_x)](1 - n_z)$$

$$= is \int d\phi(1 - n_z), \tag{7.105}$$

which is rather analogous to the coordinate-dependent expression in Equation (7.79).

It was already noted from Equation (7.93) that ϕ has to be imaginary. To recover the quantum-phase interference in the coordinate-independent formalism, ϕ must be translated from the initial point, say $\phi = 0$, to the final point, $\phi = n\pi + i\phi_I$, $n = 0, 1$ before and after the instanton occurs [99]. The two contributions to the action from these paths are given by

$$S_{WZ}^I = is \int_0^{\pi + i\phi_I} d\phi(1 - n_z)|_{n_z=1} + is \int_{\pi + i\phi_I}^0 d\phi(1 - n_z)|_{n_z=-1}$$

$$= -2\pi is + 2s\phi_I \tag{7.106}$$

and

$$S_{WZ}^{II} = is \int_0^{i\phi_I} d\phi(1 - n_z)|_{n_z=1} \tag{7.107}$$

$$+ is \int_{i\phi_I}^0 d\phi(1 - n_z)|_{n_z=-1} = 2s\phi_I$$

which are exactly the expressions as before. Then the previous evaluation quantum interference goes through unchanged.

7.7 Instantons in the Spin Exchange Model

We will study a second example where instantons give rise to quantum tunnelling in spin systems and breaks the degeneracy, the case of two large, coupled, quantum spins in the presence of a large, simple, easy-axis anisotropy, interacting with each other through a standard spin–spin exchange coupling, corresponding to the Hamiltonian

$$H = -K(S_{1z}^2 + S_{2z}^2) + \lambda \vec{S}_1 \cdot \vec{S}_2. \tag{7.108}$$

We will take $K > 0$ and the case of equal spins $\vec{S}_1 = \vec{S}_2 = \vec{S}$. $\lambda > 0$ gives an anti-ferromagnetic coupling while $\lambda < 0$ sign corresponds to ferromagnetic coupling. The first term gives rise to the anisotropy, favouring an easy-axis, the z-axis, the first term's contribution to the energy is obviously minimized if the spin is pointing along the z-direction and is as large as possible. The second term is called the Heisenberg exchange energy interaction. The spins $\vec{S}_i$ could correspond to quantum spins of macroscopic multi-atomic molecules [113, 116, 90], or the quantum spins of macroscopic ferromagnetic grains [28, 27], or the average spin of each of the two staggered Néel sub-lattices in a quantum anti-ferromagnet [116, 91, 92].

A Néel lattice is simply a spin system where adjacent spins are maximal and point in opposite directions. It is the epitome of anti-ferromagnetic order. We will be exclusively looking at one dimension, thus what are called spin chains. As the spins on a lattice are distinguishable, one choice starting at a given spin of up, down, up, down, $\cdots$ is a different configuration from down, up, down, up, $\cdots$, starting from the same spin. This twofold degeneracy is akin to the two-fold degeneracy of a ferromagnetic system, where all spins could point up or all spins could point down. The direction of the up and down is determined by the anisotropy, which picks out a favoured direction for the spins. In this section, we will only consider two spins, but in the next section we will generalize our results to a spin chain.

The non-interacting system of our Hamiltonian is defined by $\lambda = 0$, here the spin eigenstates of S_{iz}, notationally $|s, s_{1z}\rangle \otimes |s, s_{2z}\rangle \equiv |s_{1z}, s_{2z}\rangle$, are obviously exact eigenstates. The ground state is fourfold degenerate, corresponding to the states $|s, s\rangle$, $|-s, -s\rangle$, $|s, -s\rangle$ and $|-s, s\rangle$, which we will write as $|\uparrow, \uparrow\rangle, |\downarrow, \downarrow\rangle, |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle$, each with energy $E = -2Ks^2$. The first excited state, which is eightfold degenerate, is split from the ground state by energy $\Delta E = K(2s - 1)$.

In the weak coupling limit, $\lambda/K \to 0$, an interesting question to ask is what is the ground state and the first few excited states of the system for large spin $\vec{S}$. For spin 1/2, the exact eigenstates are trivially found; for spin 1, the problem is a 9×9 matrix, which again can be diagonalized, but for the general case we must diagonalize a $(2s + 1)^2 \times (2s + 1)^2$ matrix, although that is rather sparse. For weak coupling the anisotropic potential continues to align or anti-align the spins along the z-axis in the ground state.

As the non-interacting ground state is fourfold degenerate, in first-order degenerate perturbation theory, we should diagonalize the exchange interaction in the degenerate subspace. However, it turns out to be already diagonal in that subspace. The full Hamiltonian can be alternatively written as

$$H = -K(S_{1z}^2 + S_{2z}^2) + \lambda\left(S_{1z}S_{2z} + \frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+)\right), \qquad (7.109)$$

where $S_i^\pm = S_{ix} \pm iS_{iy}$ for $i = 1, 2$. $S_i^\pm$ act as raising and lowering operators for S_{iz}, and hence they must annihilate the states $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$. Thus the two states $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$ are actually exact eigenstates of the full Hamiltonian with exact energy eigenvalue $(-2K + \lambda)s^2$. These two states do not mix with the two states $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$ as the eigenvalue of $S_{1z} + S_{2z}$, which is conserved, is $+2s, -2s$ for the two ferromagnetic states and 0 for the two anti-ferromagnetic states. The perturbation, apart from the diagonal term $\lambda S_{1z}S_{2z}$, acting on the two states $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$ takes them out of the degenerate subspace, thus this part does not give any correction to the energy. The action of the diagonal term on either of these states is equal to $-\lambda s^2$. Thus the perturbation corresponds to the identity matrix within the degenerate subspace of the two states $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$, with eigenvalue $-\lambda s^2$ for the two anti-ferromagnetic states. This yields, in first-order degenerate perturbation theory, the perturbed energy eigenvalue of $(-2K - \lambda)s^2$ for the two states $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$. Thus the following picture emerges of the first four levels in first-order degenerate perturbation theory. For the $\lambda < 0$ (ferromagnetic coupling), the states $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$ are the exact, degenerate ground states of the theory, with energy eigenvalue $(-2K + \lambda)s^2 = (-2K - |\lambda|)s^2$. The first excited states are also degenerate, but only within first-order degenerate perturbation theory. They are given by $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$, with energy eigenvalue $(-2K - \lambda)s^2 = (-2K + |\lambda|)s^2$. For the $\lambda > 0$ (anti-ferromagnetic coupling), the roles are exactly reversed. The states $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle$ give the degenerate ground state with energy $(-2K - \lambda)s^2$ in first-order degenerate perturbation, while the states $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$ give the exact, first (doubly degenerate) excited level with energy $(-2K + \lambda)s^2$. Thus the Hamiltonian in first-order degenerate perturbation theory is simply diagonal

$$\langle H \rangle = \begin{pmatrix} -2K + \lambda & 0 & 0 & 0 \\ 0 & -2K + \lambda & 0 & 0 \\ 0 & 0 & -2K - \lambda & 0 \\ 0 & 0 & 0 & -2K - \lambda \end{pmatrix} s^2 \qquad (7.110)$$

in the ordered basis $\{|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle\}$. The two ferromagnetic states are the exact degenerate ground states for $\lambda < 0$, while the two anti-ferromagnetic states are the approximate ground states for $\lambda > 0$.

However, we do not expect this result to stand in higher orders. We will show that, in fact, the states $|\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle \pm |\downarrow\uparrow\rangle)$ are the appropriate linear combinations implied by higher orders in degenerate perturbation theory, for the

ground state in the anti-ferromagnetic case, and they are the second and third excited states in the ferromagnetic case. We will also show that the states $|\pm\rangle$ are no longer degenerate. The perturbing Hamiltonian links the state $|\pm s, \mp s\rangle$ only to the state $|\pm s \mp 1, \mp s \pm 1\rangle$. To reach the state $|\mp s, \pm s\rangle$ from the state $|\pm s, \mp s\rangle$ requires one to go to $2s$th order in perturbation, and s is assumed to be large. Indeed, we find our results via macroscopic quantum tunnelling using the spin-coherent state path integral. Using the path integral to determine large orders in perturbation theory has already been studied in field theory [35, 128].

Our two-spin system, in Minkowski time, is governed by an action $S = \int dt \mathcal{L}$ where,

$$\mathcal{L} = \int dx\, s\hat{n}_1 \cdot (\partial_x \hat{n}_1 \times \partial_t \hat{n}_1) - V_1(\hat{n}_1)$$

$$+ \int dx\, s\hat{n}_2 \cdot (\partial_x \hat{n}_2 \times \partial_t \hat{n}_2) - V_2(\hat{n}_2) - \lambda \hat{n}_1 \cdot \hat{n}_2, \qquad (7.111)$$

where now $\hat{n}_i = (\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i)$, $i = 1, 2$ are two different 3-vectors of unit norm, representing semi-classically the quantum spin [28, 27] and s is the value of each spin. We use the coordinate-dependent spherical-polar coordinate to describe the spins and the Lagrangian takes the form

$$\mathcal{L} = -s\dot{\phi}_1(1 - \cos\theta_1) - V_1(\theta_1, \phi_1)$$

$$-s\dot{\phi}_2(1 - \cos\theta_2) - V_2(\theta_2, \phi_2)$$

$$-\lambda\left(\sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2) + \cos\theta_1 \cos\theta_2\right). \qquad (7.112)$$

Our analysis is valid if we restrict our attention to any external potential with easy-axis, azimuthal symmetry, with a reflection symmetry (along the azimuthal axis), as in [68], $V_i(\theta_i, \phi_i) \equiv V(\theta_i) = V(\pi - \theta_i)$, $i = 1, 2$. The potential is further assumed to have a minimum at the north pole and the south pole, at $\theta_i = 0$, and π. We will treat the special simple case of the potential given by

$$V(\hat{n}_i) \equiv V(\theta_i, \phi_i) = K\sin^2\theta_i. \qquad (7.113)$$

corresponding exactly to our Hamiltonian Equation (7.108). It was shown in [68], for uncoupled spins, that quantum tunnelling between the spin up and down states of each spin separately is actually absent because of conservation of the z-component of each spin. With the exchange interaction, only the total z-component is conserved, allowing transitions $|\uparrow, \downarrow\rangle \longleftrightarrow |\downarrow, \uparrow\rangle$. In general, tunnelling exists if there is an equipotential path that links the beginning and end points. We will see that such an equipotential path exists, but through complex values of the phase space variables.

We must find the critical points of the Euclidean action with $t \rightarrow -i\tau$, which gives

$$\mathcal{L}_E = is\dot{\phi}_1(1 - \cos\theta_1) + V(\theta_1) + is\dot{\phi}_2(1 - \cos\theta_2) + V(\theta_2)$$

$$+ \lambda\left(\sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2) + \cos\theta_1 \cos\theta_2\right). \qquad (7.114)$$

The solutions must start at $(\theta_1, \phi_1) = (0,0)$ and $(\theta_2, \phi_2) = (\pi, 0)$, say, and evolve to $(\theta_1, \phi_1) = (\pi, 0)$ and $(\theta_2, \phi_2) = (0,0)$. In Euclidean time, the WZ term has become imaginary and the equations of motion in general only have solutions for complexified field configurations. Varying with respect to ϕ_i gives equations that correspond to the conservation of angular momentum:

$$is\frac{d}{d\tau}\left(1 - \cos\theta_1\right) + \lambda\sin\theta_1\sin\theta_2\sin\left(\phi_1 - \phi_2\right) = 0 \qquad (7.115)$$

$$is\frac{d}{d\tau}\left(1 - \cos\theta_2\right) - \lambda\sin\theta_1\sin\theta_2\sin\left(\phi_1 - \phi_2\right) = 0 \qquad (7.116)$$

Varying with respect to θ_i gives the equations:

$$is\dot{\phi}_1\sin\theta_1 + 2K\sin\theta_1\cos\theta_1 + \lambda\left(\cos\theta_1\sin\theta_2\cos(\phi_1 - \phi_2) - \sin\theta_1\cos\theta_2\right) = 0 \qquad (7.117)$$

$$is\dot{\phi}_2\sin\theta_2 + 2K\sin\theta_2\cos\theta_2 + \lambda\left(\cos\theta_2\sin\theta_1\cos(\phi_1 - \phi_2) - \sin\theta_2\cos\theta_1\right) = 0. \qquad (7.118)$$

Adding Equations (7.115) and (7.116) we simply get

$$\frac{d}{d\tau}\left(\cos\theta_1 + \cos\theta_2\right) = 0. \qquad (7.119)$$

Hence $\cos\theta_1 + \cos\theta_2 = l = 0$, where the constant l is chosen to be zero using the initial condition $\theta_1 = 0, \theta_2 = \pi$ and therefore we can take $\theta_2 = \pi - \theta_1$. We can now eliminate θ_2 from the equations of motion, and writing $\theta = \theta_1$, $\phi = \phi_1 - \phi_2$ and $\Phi = \phi_1 + \phi_2$ we get the effective Lagrangian:

$$\mathcal{L} = is\dot{\Phi} - is\dot{\phi}\cos\theta + U(\theta, \phi), \qquad (7.120)$$

where $U(\theta, \phi) = 2K\sin^2\theta + \lambda\left(\sin^2\theta\cos\phi - \cos^2\theta\right) + \lambda$ is the effective potential energy. We have added a constant λ so that the potential is normalized to zero at $\theta = 0$. The first term in the Lagrangian is a total derivative and drops out. The equations of motion become:

$$is\dot{\phi}\sin\theta = -\frac{\partial U(\theta, \phi)}{\partial\theta} \qquad (7.121)$$

$$is\dot{\theta}\sin\theta = \frac{\partial U(\theta, \phi)}{\partial\phi}. \qquad (7.122)$$

These equations have no solutions on the space of real functions $\theta(\tau), \phi(\tau)$ due to the explicit i on the left-hand side. The analogue of conservation of energy follows immediately from these equations, multiplying (7.121) by $\dot{\theta}$ and (7.122) by $\dot{\phi}$ and subtracting, gives:

$$\frac{dU(\theta, \phi)}{d\tau} = 0, \quad i.e. \quad U(\theta, \phi) = const. = 0. \qquad (7.123)$$

The constant has been set to 0 again using the initial condition $\theta = 0$. Thus we have, specializing to our case, Equation (7.113)

$$U(\theta, \phi) = (2K + \lambda(\cos\phi + 1))\sin^2\theta = 0 \tag{7.124}$$

implying $(2K + \lambda(\cos\phi + 1)) = 0$, since $\sin^2\theta \neq 0$, as is required for a non-trivial solution. Thus

$$\cos\phi = -\left(\frac{2K}{\lambda} + 1\right) \tag{7.125}$$

and we see that ϕ must be a constant. This is not valid in general, it is due to the specific choice of the external potential Equation (7.113). Since $K > |\lambda|$ we get $|\cos\phi| > 1$, which of course has no solution for real ϕ. We take $\phi = \phi_R + i\phi_I$ which gives $\cos\phi = \cos\phi_R \cosh\phi_I - i\sin\phi_R \sinh\phi_I$. As the right-hand side of Equation (7.125) is real, we must have either $\phi_I = 0$ or $\phi_R = n\pi$ or both. Clearly the $\phi_I = 0$ cannot yield a solution for Equation (7.125), hence we must take $\phi_R = n\pi$. As we must impose 2π periodicity on ϕ_R, only $n = 0$ or 1 exist. Then we get

$$\cos\phi = (-1)^n \cosh\phi_I = \begin{cases} -\left(\frac{2K}{\lambda} + 1\right) & \text{if } \lambda > 0 \\ +\left(\frac{2K}{|\lambda|} - 1\right) & \text{if } \lambda < 0 \end{cases}. \tag{7.126}$$

Thus $n = 1$ for $\lambda > 0$ and $n = 0$ for $\lambda < 0$ allowing for the unified expression

$$\cosh\phi_I = \frac{2K + \lambda}{|\lambda|}. \tag{7.127}$$

Equation (7.122) simplifies to

$$is\frac{\dot{\theta}}{\sin\theta} = -\lambda\sin\phi = -i\lambda(-1)^n \sinh\phi_I = i|\lambda|\sinh\phi_I \tag{7.128}$$

as $\lambda(-1)^n = -|\lambda|$. Equation (7.127) has two solutions: positive ϕ_I corresponds to the instanton, $(\dot{\theta} > 0)$, and negative ϕ_I corresponds to the anti-instanton, $(\dot{\theta} < 0)$. The equation is trivially integrated with solution

$$\theta(\tau) = 2\arctan\left(e^{\omega(\tau - \tau_0)}\right), \tag{7.129}$$

where $\omega = (|\lambda|/s)\sinh\phi_I$ and at $\tau = \tau_0$ we have $\theta(\tau) = \pi/2$, which has exactly the same form as the solution in the previous section, Equation (7.78). Thus $\theta(\tau)$ interpolates from 0 to π as τ interpolates from $-\infty$ to ∞ for an instanton and from π to 0 for an anti-instanton.

Using $\dot{\phi} = 0$ and Equation (7.123) that the effective energy is zero, we see that the action for this instanton trajectory, let us call it S_0, simply vanishes $S_0 = \int_{-\infty}^{\infty} d\tau \mathcal{L} = 0$. So where does the amplitude come from? As in the previous section, we have not taken into account the fact that ϕ must be translated from $\phi = 0$ (any initial point will do, as long as it is consistently used to compute the full amplitude) to $\phi = n\pi + i\phi_I$ before the instanton can occur and then back to

$\phi = 0$ after the instanton has occurred. Normally such a translation has no effect; either the contribution at the beginning cancels that at the end or, if the action is second-order in time derivative, moving adiabatically gives no contribution. But in the present case, for an instanton, before the instanton occurs, $\theta = 0$, while after it has occurred, $\theta = \pi$, and vice versa for an anti-instanton. As $\dot\phi$ is multiplied by $\cos\theta$ in the action, the two contributions actually add, and there is a net contribution to the action. Indeed, the full action for the combination of the instanton and the changes in ϕ is given by

$$\Delta S = \int_0^{n\pi + i\phi_I} -isd\phi\cos\theta|_{\theta=0} + S_0 + \int_{n\pi+i\phi_I}^0 -isd\phi\cos\theta|_{\theta=\pi}$$
$$= -is2n\pi + 2s\phi_I \tag{7.130}$$

we call it ΔS since it arises because of a change in ϕ, and where we have put $S_0 = 0$.

We will use this information to compute the following matrix element, using the spin-coherent states $|\theta,\phi\rangle$ and the two lowest energy eigenstates $|E_0\rangle$ and $|E_1\rangle$:

$$\langle\theta_f,\phi_f|e^{-\beta H}|\theta_i,\phi_i\rangle = e^{-\beta E_0}\langle\theta_f,\phi_f|E_0\rangle\langle E_0|\theta_i,\phi_i\rangle$$
$$+e^{-\beta E_1}\langle\theta_f,\phi_f|E_1\rangle\langle E_1|\theta_i,\phi_i\rangle + \cdots \tag{7.131}$$

On the other hand, the matrix element is given by the spin-coherent state path integral

$$\langle\theta_f,\phi_f|e^{-\beta H}|\theta_i,\phi_i\rangle = \mathcal{N}\int_{\theta_i,\phi_i}^{\theta_f,\phi_f}\mathcal{D}\theta\mathcal{D}\phi\, e^{-S_E}. \tag{7.132}$$

The integration is done in the saddle point approximation. With $(\theta_i,\phi_i) = (0,0)$ corresponding to the state $|\uparrow,\downarrow\rangle$ and $(\theta_f,\phi_f) = (\pi,0)$ corresponding to the state $|\downarrow,\uparrow\rangle$, we get

$$\langle\downarrow,\uparrow|e^{-\beta H}|\uparrow,\downarrow\rangle = \mathcal{N}e^{-\Delta S}\kappa\beta(1+\cdots), \tag{7.133}$$

where κ is the ratio of the square root of the determinant of the operator governing the second-order fluctuations about the instanton excluding the time translation zero mode, and that of the free determinant. It can, in principle, be calculated, but we will not do this here. The zero mode is taken into account by integrating over the position of the occurrence of the instanton giving rise to the factor of β. $\mathcal{N}$ is the overall normalization including the square root of the free determinant which is given by $Ne^{-E_0\beta}$, where E_0 is the unperturbed ground-state energy and N is a constant that depends on the form of the perturbative ground-state wave function. The result exponentiates, but since we must sum over all sequences of one instanton followed by any number of anti-instanton–instanton pairs, the total number of instantons and anti-instantons is odd, and we get

$$e^{-\Delta S}\kappa\beta \to \sinh\left(e^{-\Delta S}\kappa\beta\right). \tag{7.134}$$

Given $\Delta S = -is2n\pi + 2s\phi_I$ and solving Equation (7.127) for ϕ_I for $K \gg |\lambda|$

$$\phi_I = \operatorname{arccosh}\left(\frac{2K + \lambda}{|\lambda|}\right) \approx \ln\left(\frac{4K}{|\lambda|}\right) \tag{7.135}$$

gives:

$$e^{-\Delta S} = \begin{cases} e^{is2\pi - 2s\phi_I} & \text{if } \lambda > 0 = \begin{cases} \left(\frac{|\lambda|}{4K}\right)^{2s} & \text{if } s \in \mathbf{Z} \\ -\left(\frac{|\lambda|}{4K}\right)^{2s} & \text{if } s \in \mathbf{Z} + 1/2 \end{cases} \\ \left(\frac{|\lambda|}{4K}\right)^{2s} & \text{if } \lambda < 0 \end{cases} \tag{7.136}$$

Then we get

$$\langle\downarrow,\uparrow|e^{-\beta H}|\uparrow,\downarrow\rangle = \pm\left(\frac{1}{2}e^{\left(\frac{|\lambda|}{4K}\right)^{2s}\kappa\beta} - \frac{1}{2}e^{-\left(\frac{|\lambda|}{4K}\right)^{2s}\kappa\beta}\right)Ne^{-\beta E_0}, \tag{7.137}$$

where the $-$ sign only applies for the case of anti-ferromagnetic coupling with half odd integer spin, *i.e.* $\lambda > 0, s = \mathbf{Z} + 1/2$. An essentially identical analysis yields, for the persistence amplitudes

$$\langle\downarrow,\uparrow|e^{-\beta H}|\downarrow,\uparrow\rangle = \langle\uparrow,\downarrow|e^{-\beta H}|\uparrow,\downarrow\rangle$$
$$= \left(\frac{1}{2}e^{\left(\frac{|\lambda|}{4K}\right)^{2s}\kappa\beta} + \frac{1}{2}e^{-\left(\frac{|\lambda|}{4K}\right)^{2s}\kappa\beta}\right)Ne^{-\beta E_0}. \tag{7.138}$$

These calculated matrix elements can now be compared with what is expected for the exact theory:

$$\langle\downarrow,\uparrow|e^{-\beta H}|\uparrow,\downarrow\rangle = e^{-\beta(E_0 - \frac{1}{2}\Delta E)}\langle\downarrow,\uparrow|E_0\rangle\langle E_0|\uparrow,\downarrow\rangle$$
$$+ e^{-\beta(E_0 + \frac{1}{2}\Delta E)}\langle\downarrow,\uparrow|E_1\rangle\langle E_1|\uparrow,\downarrow\rangle \tag{7.139}$$

and

$$\langle\downarrow,\uparrow|e^{-\beta H}|\downarrow,\uparrow\rangle = e^{-\beta(E_0 - \frac{1}{2}\Delta E)}\langle\downarrow,\uparrow|E_0\rangle\langle E_0|\downarrow,\uparrow\rangle$$
$$+ e^{-\beta(E_0 + \frac{1}{2}\Delta E)}\langle\downarrow,\uparrow|E_1\rangle\langle E_1|\downarrow,\uparrow\rangle \tag{7.140}$$

The energy splitting can be read off from this result

$$\Delta E = E_1 - E_2 = 2\left(\frac{|\lambda|}{4K}\right)^{2s}\kappa \tag{7.141}$$

for all cases; however, the wave functions are different. The low-energy eigenstates are given by

$$|E_0\rangle = \frac{1}{\sqrt{2}}(|\downarrow,\uparrow\rangle + |\uparrow,\downarrow\rangle) \qquad |E_1\rangle = \frac{1}{\sqrt{2}}(|\downarrow,\uparrow\rangle - |\uparrow,\downarrow\rangle) \tag{7.142}$$

for the case $\lambda > 0$ for $s \in \mathbf{Z}$, where they are the actual ground and first excited state as well as for the case $\lambda < 0$ (although here these energy eigenstates should be labelled $|E_3\rangle$ and $|E_4\rangle$ as the actual ground states are the ferromagnetic states $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$). For the fermionic spin, anti-ferromagnetic case with $\lambda > 0$ and $s \in \mathbf{Z} + 1/2$ we get the reversal of the states

$$|E_0\rangle = \frac{1}{\sqrt{2}}(|\downarrow,\uparrow\rangle - |\uparrow,\downarrow\rangle) \qquad |E_1\rangle = \frac{1}{\sqrt{2}}(|\downarrow,\uparrow\rangle + |\uparrow,\downarrow\rangle), \qquad (7.143)$$

but the energy splitting remains the same.

This understanding of the ground state in the anti-ferromagnetic case is the main result. This difference in the ground states for integer and half-odd integer spins is understood in terms of the Berry phase [88, 38] (computed by the change in the WZ term) for the evolution corresponding to the instanton. It can also be understood by looking at perturbation theory to order $2s$; the details cannot be given here. Briefly, the action of the perturbation Equation (7.109) will lower one spin and raise the other. This can be done $2s$ times when we achieve a complete flip of both spins. We find that the effective 2×2 Hamiltonian for the degenerate subspace is proportional to the identity plus off-diagonal terms that are symmetric. For the integer spin case the off-diagonal terms are negative and for the half-odd integer case they are positive. Diagonalizing this 2×2 matrix gives the solutions for the ground states, exactly as we have found.

7.8 The Haldane-like Spin Chain and Instantons

The study of quantum spin chains has been a very important physical problem in condensed matter and mathematical physics over the past 100 years. They play an exemplary role in the study of strongly correlated quantum systems. In both experimental and theoretical physics, models of quantum spin chains are one of the most fundamental systems endowed with interesting phenomenon. The classic work on spin chains was that of Bethe [14] and Hulthén [63] for the one-dimensional ($D = 1$), isotropic Heisenberg spin-$\frac{1}{2}$ anti-ferromagnetic chain. They computed the exact anti-ferromagnetic ground state and its energy for an infinite chain. Anderson [6] worked out the ground-state energies and the spectrum for $D = 1, 2, 3$ by means of spin wave theory. The inclusion of an anisotropy term introduces much interesting physics ranging from quantum computing [90] to optical physics [110]. The resulting Hamiltonian is what we will study in this section. It now possesses two coupling constants which can compete against each other to lower the energy

$$\hat{H} = -K \sum_{i=1}^{N} S_{i,z}^2 + \lambda \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} \qquad (7.144)$$

and we consider the chain with periodic boundary conditions and consider $\lambda > 0$ so that we are in the anti-ferromagnetic regime, which is the more interesting regime.

This model is the generalization to a spin chain of the two-spin model that we studied in the previous section. Here each nearest-neighbour pair corresponds to the two-spin system that we have just studied. Each spin has magnitude $|\vec{S}_i| = s$ and we will consider the large s limit. The two limiting cases are weak anisotropy $\lambda \gg K$ and weak exchange coupling $\lambda \ll K$, where λ is the Heisenberg exchange interaction coupling constant and K is the anisotropy coupling constant. The limit of weak anisotropy was studied in a celebrated paper by Haldane [59] in a closely related model, hence we call our model a Haldane-like spin chain. Haldane demonstrated that in the large spin limit, $s \gg 1$, the system can be mapped to a non-linear sigma model in field theory with distinguishing effects between integer and half-odd integer spins. The full rotational symmetry is broken explicitly into rotational symmetry about the z-axis with the total z-component $S_{i,z} = \sum_i S_{i,z}$ conserved. The Hamiltonian also possesses a discrete reflection symmetry about the z-axis $S_{i,z} \to -S_{i,z}$. We will also study the model in the large spin limit, but we will take the limit of strong anisotropy, $K \gg \lambda$, the opposite limit to Haldane.

With $\lambda = 0$, the ground state is 2^N-fold degenerate, corresponding to each spin in the state $S_z = \pm s$. Then $s_z^2 = s^2$ and the energy is $-Ks^2 2N$, which is minimal. For an even number of sites, the model is called bi-partite and the two fully anti-aligned Neél states are good starting points for investigating the ground state. For an odd number of sites, the Neél states are frustrated; they must contain at least one defect, which are called domain wall solitons [115, 39, 93, 20, 95]. There is a high level of degeneracy as the soliton can be placed anywhere along the cyclic, periodic chain and this degenerate system is the starting point for investigating the ground state for the case of an odd number of sites. Frustrated systems are of great importance in condensed matter physics as they lead to exotic phases of matter such as spin liquid [9], spin glasses [15] and topological orders [73]. Solitons will also occur on the periodic chain with even number of sites, but they must occur in soliton–anti-soliton pairs.

Many physical magnetic systems such as $CsNiF_3$ and Co^{++} have been modelled with Hamiltonians of the form of Equation (7.144). Models of this form have been of research interest over the years since the work of Haldane [59]. To mention but a few, quite recently, the ground-state phase diagrams of the spin-2 XXZ anisotropic Heisenberg chain has been carefully investigated by the infinite system density-matrix-renormalization group (iDMRG) algorithm [74] and other numerical methods [58]. For the spin-1 XXZ anisotropic Heisenberg chain, the numerical exact diagonalization has been extensively investigated for finite size systems [25]. For an arbitrary spin, the phase diagrams and correlation exponents of an XXZ anisotropic Heisenberg chain has also been studied by representing the spins as a product of $2s$ spin $\frac{1}{2}$ operators [108]. This

research has been focussed on ground-state phase diagrams and the existence of Haldane phase (conjecture). In this section, we will study the spin chain with Hamiltonian given by the simple form given in Equation (7.144) with periodic boundary condition $\vec{S}_{N+1} = \vec{S}_1$, and we consider $K \gg \lambda > 0$, *i.e.* strong easy-axis anisotropy and perturbative Heisenberg anti-ferromagnetic coupling. In the first subsection, we will study macroscopic quantum tunnelling of the Hamiltonian-defined Equation (7.144) for the case of an even spin chain. This analysis is based on spin-coherent state path integral formalism, which is appropriate for large spin systems. In the second subsection, which we include for completeness, we will deal with the case of an odd spin chain. Here, spin-coherent state path integral formalism fails to give a definitive result. Thus, our analysis is based on perturbation theory.

7.8.1 Even Number of Sites and Spin-Coherent State Path Integral

Let us consider our model, Equation (7.144), for N even. The ground state of the free theory (K term) is 2^N-fold degenerate corresponding to each spin in the highest (lowest) weight states $m = \pm s$. In the degenerate subspace, there are two fully aligned states $|\uparrow,\uparrow,\uparrow,\uparrow,\cdots,\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow,\downarrow,\downarrow,\cdots,\downarrow,\downarrow\rangle$ and two fully anti-aligned Neél states $|p\rangle = |\uparrow,\downarrow,\uparrow,\downarrow,\cdots,\uparrow,\downarrow\rangle$ and $|-p\rangle = |\downarrow,\uparrow,\downarrow,\uparrow,\cdots,\downarrow,\uparrow\rangle$, where the arrow denotes the highest (lowest) weight states, *i.e.* $m = s \equiv\uparrow (m = -s \equiv\downarrow)$ for each individual spin and the remaining degenerate states are produced by flipping individual spins relative to these extremal states. These two Neél states $|\pm p\rangle$ have the lowest energy at first-order in perturbation theory; however, they are not exact eigenstates of the quantum Hamiltonian in Equation (7.144), thus we expect ground-state quantum tunnelling coherence between them. Such tunnelling is usually mediated by an instanton trajectory, and the exponential of the instanton action (multiplied by a prefactor) yields the energy splitting. We will obtain this instanton trajectory via the spin-coherent state path integral formalism [5, 76, 75, 99], which is the appropriate formalism for large spin systems. In this formalism, the spin operators become unit vectors parameterized by spherical coordinates. The corresponding Euclidean Lagrangian in this formalism is given by

$$L_E = is \sum_{i=1}^{N} \dot{\phi}_i (1 - \cos\theta_i) + K \sum_{i=1}^{N} \sin^2\theta_i$$

$$+ \lambda \sum_{i=1}^{N} \left(\sin\theta_i \sin\theta_{i+1} \cos(\phi_i - \phi_{i+1}) + \cos\theta_i \cos\theta_{i+1} \right), \qquad (7.145)$$

where the periodicity condition $i = N + 1 = 1$ is imposed. The first term is the usual WZ [120] term which arises from the non-orthogonality of spin-coherent states while the other two terms correspond to the anisotropy energy and the Heisenberg exchange energy. Quantum amplitudes are obtained via the path integral and the saddle point approximation. Solutions of the Euclidean classical

equations of motion give information about quantum tunnelling amplitudes. The Euclidean classical equation of motion for ϕ_i is

$$is\frac{d(1-\cos\theta_i)}{d\tau} = \sin\theta_{i-1}\sin\theta_i\sin(\phi_{i-1}-\phi_i)$$
$$-\sin\theta_i\sin\theta_{i+1}\sin(\phi_i-\phi_{i+1}) \tag{7.146}$$

while the equation of motion for θ_i is

$$0is\dot\phi_i\sin\theta_i + 2K\sin\theta_i\cos\theta_i$$
$$\lambda(\cos\theta_i(\sin\theta_{i+1}\cos(\phi_i-\phi_{i+1})) + \sin\theta_{i-1}\cos(\phi_{i-1}-\phi_i))$$
$$= \lambda(\sin\theta_i(\cos\theta_{i+1}+\cos\theta_{i-1})) = 0. \tag{7.147}$$

Summing both sides of Equation (7.146) gives

$$is\sum_i\frac{d(1-\cos\theta_i)}{d\tau} = 0 \Rightarrow \sum_i\cos\theta_i = l = 0, \tag{7.148}$$

which corresponds to the conservation of the z-component of the total spin $\sum_i S_i^z$, as the full Hamiltonian, Equation (7.144), is invariant under rotations about the z-axis.

We will solve these equations using simplifying, physically motivated ansatze. A particular solution of Equation (7.148) is $\theta_{2k-1} \equiv \theta$, and $\theta_{2k} = \pi - \theta$, $k = 1, 2\cdots, N/2$. Making the further simplifying ansatz $\phi_i - \phi_{i+1} = (-1)^{i+1}\phi$ effectively reducing the system to a single spin problem, we get the effective Lagrangian (adding an irrelevant constant)

$$L_E^{eff} = is\sum_{k=1}^N\dot\phi_k - is\cos\theta\sum_{k=1}^{N/2}(\dot\phi_{2k-1}-\dot\phi_{2k})$$
$$+\sum_{i=1}^N\left[K+\lambda[1+\cos(\phi_i-\phi_{i+1})]\right]\sin^2\theta \tag{7.149}$$

$$= isN\dot\Phi - \frac{isN}{2}\dot\phi\cos\theta + U_{eff}, \tag{7.150}$$

where $U_{eff} = N[K+\lambda(1+\cos\phi)]\sin^2\theta$. The spin chain problem has reduced to essentially the same problem we studied in the previous section with just two spins. The instanton that we will find must go from $\theta = 0$ to $\theta = \pi$. Conservation of energy implies $\partial_\tau U_{eff} = 0$, which then must vanish, $U_{eff} = 0$, since it is so at $\theta = 0$. This implies

$$\cos\phi = -\left(\frac{K}{\lambda}+1\right) \ll -1 \tag{7.151}$$

since $\sin\theta(\tau) \neq 0$ along the whole trajectory. Thus ϕ is a complex constant which can be written as $\phi = \pi + i\phi_I$ identical to that of the two-spin case [99]. The classical equation of motion for ϕ gives

$$is\dot\theta = -2\lambda\sin\theta\sin\phi = i2\lambda\sin\theta\sinh\phi_I \tag{7.152}$$

which integrates as

$$\theta(\tau) = 2\arctan\left(e^{\omega(\tau-\tau_0)}\right), \tag{7.153}$$

where $\omega = (2\lambda/s)\sinh\phi_I$. The instanton is independent of the number of spins and only depends on the initial and the final points. As found in [99], the instanton contributes to the action only through the WZ term, as $U_{eff} = 0$ all along the trajectory. The action is given by [99]

$$S_c = S_0 - \frac{isN}{2}\int_0^{\pi+i\phi_I} d\phi\cos\theta|_{\theta=0} - \frac{isN}{2}\int_{\pi+i\phi_I}^0 d\phi\cos\theta|_{\theta=\pi}$$
$$= 0 - isN\pi + Ns\phi_I = -isN\pi + Ns\phi_I. \tag{7.154}$$

The two Neél states reorganize into the symmetric and anti-symmetric linear superpositions, $|+\rangle$ and the $|-\rangle$ as in [99]. The energy splitting is then

$$\Delta E = 2\mathcal{D}e^{-S_c} = 2\mathcal{D}\left(\frac{\lambda}{2K}\right)^{Ns}\cos(sN\pi) \tag{7.155}$$

where $\mathcal{D}$ is a determinantal pre-factor which contains no λ dependence. The factor of λ^{Ns} signifies that this energy splitting arises from $2s\left(\frac{N}{2}\right)$ order in degenerate perturbation theory in the interaction term. The energy splitting, Equation (7.155), is the general formula for any even spin chain N. For $N = 2$, we recover the results obtained previously [29, 30, 71, 72, 99]. The factor sN can be even or odd, depending on the value of the spin. For half-odd integer spin $(2l+1)/2$ and for $N = 2(2k+1)$, the argument of the cosine in Equation (7.155) is $sN\pi = (2l+1)(2k+1)\pi$ and hence we find ΔE is negative, which means that $|-\rangle$ is the ground state and $|+\rangle$ is the first excited state. In all other cases, for any value of the spin s and $N = 2(2k)$ the argument of the cosine is $sN\pi = (2s)(2k)\pi$, which is an even integer multiple of π and hence we find ΔE is positive and then $|+\rangle$ is the ground state, $|-\rangle$ is the first excited state.

7.8.2 Odd Spin Chain, Frustration and Solitons

We include the analysis of the spin chain with an odd number of sites for the sake of completeness. This system can, in principle, be analysed using the spin-coherent state path integral. However, the tunnelling transitions are quite different, and no explicit, analytic expressions for the instantons that are required are known. In this situation, we revert back to the calculation using perturbative methods, which is actually quite interesting.

When we consider a periodic chain with an odd number of sites, a soliton-like defect arises due to the spin frustration. The fully anti-aligned Neél-like state cannot complete periodically, as it requires an even total number of spins. Thus there has to be at least one pair of spins that is aligned. This can come in the form up–up or down–down while all other pairs of neighbouring spins are in the up–down or down–up combination. As the total z-component of the

spin is conserved, these states lie in orthogonal super-selection sectors and never transform into each other. The position of the soliton is arbitrary thus each sector is N-fold degenerate. In the first case the total z-component of the spin is s while in the second case it is $-s$. We will, without loss of generality, consider the s sector. These degenerate states are denoted by $|k\rangle$, $k = 1, \cdots, N$, where

$$|k\rangle = |\uparrow, \downarrow, \uparrow, \downarrow, \uparrow, \cdots, \underbrace{\uparrow, \uparrow,}_{k, k+1 th\, \text{place}}, \cdots, \uparrow, \downarrow\rangle \qquad (7.156)$$

in obvious notation. These states are not exact eigenstates of the quantum spin Hamiltonian in Equation (7.144), thus we also expect ground-state quantum tunnelling amongst these states, just as in the case of a particle in a periodic potential, which would lift the degeneracy and reorganize the soliton states into a band. The explicit form of the required instanton, which from the spin-coherent state path integral would give rise to the appropriate tunnelling, is not known. However, from Equation (7.155) we can see for the case of even spins that energy splitting actually arises at the $2s \left(\frac{N}{2} \right)$ order in (degenerate) perturbation theory. The path integral and instanton method only gives the result which must also be available at this high order in degenerate perturbation theory. This indicates that the appropriate formalism for the odd quantum spin chain would simply be (degenerate) perturbation theory at high order.

It is convenient to write the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V} \qquad (7.157)$$

where $\hat{H}_0$ represents the K (free) term and $\hat{V}$ represents the λ (perturbative) term. The states in Equation (7.156) all have the same energy $E_s = -KNs^2$ from $\hat{H}_0$ and in first-order degenerate perturbation theory $E_s = -KNs^2 - \lambda(N-1)s^2 + \lambda s^2 = (-K - \lambda)Ns^2 + 2\lambda s^2$ and are split from the first excited level, which requires the introduction of a soliton/anti-soliton pair, by an energy of 4λ. As we take the limit $K \gg \lambda$, we assume that the action of lowering or raising the value of $\hat{S}_z$ incurs an energy cost proportion to K which is much more energy than creating a soliton/anti-soliton pair, which has an energy cost proportional to λ. Although the soliton/anti-soliton states are the next states in the spectrum, they cannot be attained perturbatively, except at order $2s$ in perturbation theory. In each order of perturbation theory less than $2s$, the degenerate multiplet of states mixes with the states of much higher energy, but due to invariance under translation, the corrections brought to each state are identical and their degeneracy cannot be split. However, at order $2s$, the degenerate multiplet is mapped to itself. Although the state of an additional soliton/anti-soliton pair is also reached at this order, since it is not degenerate in energy with the original multiplet of N states, its correction will be perturbatively small.

Reaching the degenerate multiplet at order $2s$ causes the multiplet to split in energy and the states to reorganize into a band. Indeed, $\hat{V}^{2s}$ contains the term

$(S_{k+1}^- S_{k+2}^+)^{2s}$ and $(S_{k-1}^+ S_k^-)^{2s}$. These operators represent quantum fluctuations close to the position of the soliton, which when acting on the ket $|k\rangle$, flips the anti-aligned pair of spins at positions $k+1, k+2$ and at $k-1, k$, respectively. It is easy to see that flipping this pair of spins has the effect of translating the soliton $|k\rangle \to |k+2\rangle$ and $|k\rangle \to |k-2\rangle$, respectively. All other terms in $\hat{V}^{2s}$ are quantum fluctuations away from the position of the soliton. They map to states out of the degenerate subspace, either inserting a soliton/anti-soliton pair or changing the value of S^z to non-extremal values, and hence do not contribute to breaking the degeneracy.

To compute the splitting and the corresponding eigenstates, we follow [30]. We have to diagonalize the $N \times N$ matrix with components $b_{\mu,\nu}$ given by

$$b_{\mu,\nu} = \langle \mu | \hat{V} \mathcal{A}^{2s-1} | \nu \rangle, \quad \mu, \nu = 1, 2, \cdots, N \quad (7.158)$$

where $\mathcal{A}^{2s-1} = \left(\frac{\mathcal{Q}}{E_s - \hat{H}_0} \hat{V} \right)^{2s-1}$, and $\mathcal{Q} = 1 - \sum |\mu\rangle \langle \mu|$. These matrices are a generalization of the 2×2 matrix in [30]. The calculation of the components is straightforward, for example, looking at $b_{\mu,1}$ we find

$$b_{\mu,1} = \left(\frac{\lambda}{2} \right)^{2s} \langle \mu | S_2^- S_3^+ \left(\frac{\mathcal{Q}}{E_s - \hat{H}_0} S_2^- S_3^+ \right)^{2s-1} | 1 \rangle$$
$$+ \left(\frac{\lambda}{2} \right)^{2s} \langle \mu | S_N^+ S_1^- \left(\frac{\mathcal{Q}}{E_s - \hat{H}_0} S_N^+ S_1^- \right)^{2s-1} | 1 \rangle. \quad (7.159)$$

Applying the operators $2s$ times on the right-hand side we obtain

$$b_{\mu,1} = \mathcal{C}[\langle \mu | 3 \rangle + \langle \mu | N-1 \rangle], \quad (7.160)$$

where $\mathcal{C}$ is given by

$$\mathcal{C} = \pm \left(\frac{\lambda}{2} \right)^{2s} \prod_{m=1}^{2s} m(2s - m + 1) \prod_{m=1}^{2s-1} \frac{1}{Km(2s-m)}$$
$$= \pm K \left(\frac{\lambda}{2K} \right)^{2s} \left[\frac{(2s)!}{(2s-1)!} \right]^2 = \pm 4Ks^2 \left(\frac{\lambda}{2K} \right)^{2s}. \quad (7.161)$$

The first product in Equation (7.161) comes from the two square roots that accompany the action of the raising and lowering operators, and the second product is a consequence of the energy denominators. The plus or minus sign arises because we have $2s - 1$ products of negative energy denominators in Equation (7.159), so if s is integer, $2s-1$ is odd and we get a minus sign, while for half-odd integer s, $2s-1$ is even and we get a plus sign. Similarly, we can show that $b_{\mu,\nu} = \mathcal{C}[\langle \mu | \nu+2 \rangle + \langle \mu | \nu-2 \rangle]$, defined periodically of course. Thus we

find that the matrix, $[b_{\mu,\nu}]$, that we must diagonalize is a circulant matrix [37]

$$[b_{\mu,\nu}] = \mathcal{C} \begin{pmatrix} 0 & 0 & 1 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & 1 & 0 & \ddots & \cdots & \ddots & \\ 1 & \cdots & \ddots & \cdots & 0 & 0 & 0 \\ 0 & 1 & \cdots & 1\cdots & 0 & 0 & 0 \end{pmatrix}. \tag{7.162}$$

In this matrix each row element is moved one step to the right, periodically, relative to the preceding row. The eigenvalues and eigenvectors are well known. The jth eigenvalue is given by

$$\varepsilon_j = b_{1,1} + b_{1,2}\omega_j + b_{1,3}\omega_j^2 + \cdots + b_{1,N}\omega_j^{N-1}, \tag{7.163}$$

where $\omega_j = e^{i\frac{2\pi j}{N}}$ is the jth, N^{th} root of unity with corresponding eigenvector $|\frac{2\pi j}{N}\rangle = (1, \omega_j, \omega_j^2, \cdots, \omega_j^{N-1})^T$, for $j = 0, 1, 2, \cdots, N-1$. For our matrix, Equation (7.162), the only non-zero coefficients are $b_{1,3}$ and $b_{1,N-1}$, thus the one-soliton energy bands are

$$\varepsilon_j = \mathcal{C}(\omega_j^2 + \omega_j^{N-2}) = \mathcal{C}(\omega_j^2 + \omega_j^{-2})$$
$$= 2\mathcal{C}\cos\left(\frac{4\pi j}{N}\right). \tag{7.164}$$

Introducing the Brillouin zone momentum $q = j\pi/N$, the energy bands Equation (7.164) can be written as

$$\varepsilon_q = 2\mathcal{C}\cos(4q) \tag{7.165}$$

which is gapless but is doubly degenerate as the cosine passes through two periods in the Brillouin zone. The exact spectrum is symmetric about the value $N/2$. With $[x]$ the greatest integer not greater than x, the states for $j = [N/2] - k$ and $j = [N/2] + k + 1$ for $k = 0, 1, 2, \cdots, [N/2] - 1$ are degenerate as $\cos\left(\frac{4\pi([N/2]-k)}{N}\right) = \cos\left(\frac{4\pi([N/2]+k+1)}{N}\right)$ since $[N/2] = N/2 - 1/2$. However, the state with $k = [N/2]$ is not paired, only $j = 0$ is allowed. When s is an integer, $\mathcal{C}$ is negative and the unpaired state $j = 0$ is the ground state which is then non-degenerate, but for s a half-odd integer, $\mathcal{C}$ is positive, and the ground states are the degenerate pair with $j = [N/2], [N/2] + 1$ in accordance with Kramers' theorem [78]. However, in the thermodynamic limit, $N \to \infty$, the spectrum simply becomes doubly degenerate for all values of the spin and gapless.