The Haldane-like Spin Chain in the Strong Anisotropy Limit

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Haldane like spin chain

- We study a periodic chain of spins, in the large spin limit with Hamiltonian:

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

- The coupling constant K is assumed to be large, compared to λ. This is the opposite limit from what Haldane took in his seminal paper:

$$H = |J| \sum_n [\vec{S}_n \cdot \vec{S}_{n+1} + \lambda S_n^z S_{n+1}^z + \mu (S_n^z)^2]$$

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- For zero coupling, the ground state is 2^N fold degenerate, with each spin being fully up or fully down along the z axis.

- With the added exchange interaction, the spin chain tries to assume a Néel state.

- For an even number of spins, this is possible without frustration, but for an odd number of spins, there must be at least one defect in the Néel order.

- We find the low lying excitations of the even and odd spin cases remarkably different.

The spin coherent states path integral

- We use the path integral to compute transition amplitudes:

$$\langle \psi | e^{-\beta H} | \chi \rangle = \int \mathcal{D}\{\theta_i, \phi_i\} \, e^{-S_E}$$

- Where the Euclidean action is given by:

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

$$+ \lambda \sum_i [\sin\theta_i \sin\theta_{i+1} \cos(\phi_i - \phi_{i+1}) + \cos\theta_i \cos\theta_{i+1}]$$

- The Feynman path integral in Minkowski space is not a well defined mathematical expression.

- The integral is not absolutely convergent.

- Consider the two dimensional example:

$$\int dx dy e^{i(x^2+y^2)}$$

Changing variables to polar coordinates we have

$$2\pi \int_0^\infty dr r e^{ir^2} = (\pi/i)e^{ir^2}\big|_0^\infty = \infty$$

- The actual definition of the path integral is via the Euclidean path integral, with imaginary time.

$$iS_{Mink.} \rightarrow -S_E$$

$$t \rightarrow -i\tau$$

$$\partial_t \rightarrow i\partial_\tau$$

$$\partial_t \phi \partial_t \phi \rightarrow -\partial_\tau \phi \partial_\tau \phi$$

$$
\begin{aligned}
iS_{Mink.} &= i \int dt\, d^d x\, (1/2)\partial_\mu \phi \partial^\mu \phi - V(\phi) \\
&= i \int dt\, d^d x\, (1/2)\partial_t \phi \partial_t \phi - (1/2)\partial_i \phi \partial_i \phi - V(\phi) \\
&\to i(-i) \int d\tau\, d^d x\, - (1/2)\partial_\tau \phi \partial_\tau \phi - (1/2)\partial_i \phi \partial_i \phi - V(\phi) \\
&\equiv -S_E
\end{aligned}
$$

- Then the Euclidean functional integral defined by:

$$
Z_E[J] = \frac{1}{\mathcal{N}} \int \mathcal{D}\phi \; e^{-S_E[\phi] + \int J\phi}
$$

- sometimes the Euclidean action is complex

- such terms are linear in the time derivative

- hence the i in front of the Minkowski space action is not cancelled, indeed:

$$\int dt\, \partial_t \longrightarrow \int d\tau\, \partial_\tau$$

thus the Euclidean action is in general complex and the functional integral is of the form:

$$Z_E = \frac{1}{\mathcal{N}} \int \mathcal{D}\phi \; e^{-S_E[\phi] + iS_{top.}[\phi]}$$

- This is not an great problem to the proper mathematical definition of the functional integral.

- However, the usual perturbative paradigm of quantum mechanics, to find the classical critical points of the action and quantize the small oscillations, is not straightforward.

- Imagine that we have written the action strictly in terms of real fields, which is always possible.

- There are, in general, no solutions to the equations of motion.

- Classical solutions are the critical points of the action.

- The corresponding equations of motion have no solution for real fields in general

- Solutions may exist, but they are off the real axis in complexified field space.

$$\frac{\delta S_E}{\delta \phi} + i \frac{\delta S_{top.}}{\delta \phi} = 0$$

Even number of sites

- This case admits the Néel states as reasonable approximations to the vacuum.

- However, they can tunnel into each other.

- The classical equation of motion is:

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

$$- \sin\theta_i\sin\theta_{i+1}\sin(\phi_i - \phi_{i+1})$$

- This equation admits a first integral:

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

- We take the solution:

$$\theta_{2k} = \pi - \theta \qquad \theta_{2k-1} \equiv \theta$$

- Which gives:

$$L_E^{eff} = is \sum_{k=1}^{N} \dot{\phi}_k - is \cos\theta \sum_{k=1}^{N/2} (\dot{\phi}_{2k-1} - \dot{\phi}_{2k})$$

$$+ \sum_{i=1}^{N} \left[K + \lambda[1 + \cos(\phi_i - \phi_{i+1})] \right] \sin^2\theta$$

- Making the further ansatz: $\phi_i - \phi_{i+1} = (-1)^{i+1}\phi$

- This gives the Lagrangian:

$$L_E^{eff} = isN\dot{\Phi} - \frac{isN}{2}\dot{\phi}\cos\theta + U_{eff}$$

- where

$$U_{eff} = N[K + \lambda(1 + \cos\phi)]\sin^2\theta$$

- Thus the N spin Hamiltonian reduces down to a single effective spin degree of freedom.

- Conservation of energy gives: $\partial_\tau U_{eff} = 0$

- which implies:

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

- The solution is $\phi = \pi + i\phi_I$

- with $\cosh \phi_I = \left(\dfrac{K}{\lambda} + 1 \right)$

- And the θ equation is:

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

- with solution $\theta(\tau) = 2 \arctan \left(e^{\omega(\tau - \tau_0)} \right) , \ \omega = (2\lambda/s) \sinh \phi_I$

- This solution is irrelevant, its action is zero.

- The action comes from the complex $\phi = \pi + i\phi_I$

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

$$= 0 - isN\pi + Ns\phi_I = -isN\pi + Ns\phi_I$$

- Thus we need:
$$\phi_I = \operatorname{arccosh}\left(\frac{K}{\lambda} + 1\right)$$
$$\approx 2\ln\left(\frac{K}{\lambda}\right)$$

- This gives
$$S_c = -isN\pi + Ns\ \ln\left(\frac{2K}{\lambda}\right)$$

- The energy splitting is then given by:
$$\Delta = 2\mathscr{D}e^{-S_c} = 2\mathscr{D}\left(\frac{\lambda}{2K}\right)^{Ns}\cos(sN\pi)$$

- This is negative for N=2(2k+1) and half odd integer spin, but otherwise positive.

- This gives the ground state is symmetric superposition of the two Néel states $|+\rangle$ for all values except $N=2(2k+1)$ and half odd integer spins, for which it is the anti-symmetric superposition $|-\rangle$.

- The dependence on the coupling constant λ^{Ns} indicates that the result can be obtained in high orders in perturbation theory.

- In the thermodynamic limit, the two Néel states become degenerate showing parity is spontaneously broken.

Odd number of sites

- The previous description is markedly different when one considers an odd number of sites.

- Here the Néel state is frustrated, there is necessarily a defect.

- As the position of the defect is arbitrary, the ground state is N fold degenerate.

$$| \, k \rangle = | \uparrow, \downarrow, \uparrow, \downarrow, \uparrow, \cdots, \underbrace{\uparrow, \uparrow,}_{k,k+1^{th} \text{ place}}, \cdots, \uparrow, \downarrow \, \rangle$$

$$\uparrow, \downarrow, \uparrow, \uparrow, \downarrow, \uparrow, \downarrow \longrightarrow \uparrow, \downarrow, \uparrow, \downarrow, \uparrow, \uparrow, \downarrow$$
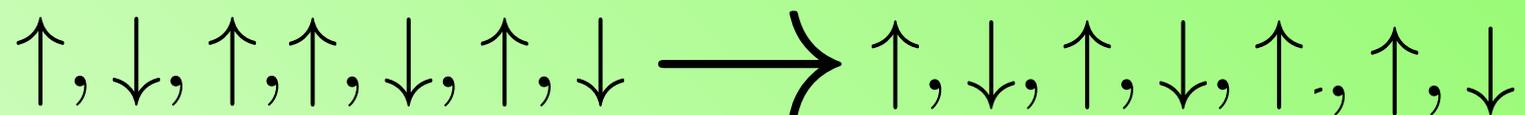
- Tunnelling allows the state $|k\rangle$ to mix with other such states.

- We tried to find the instanton that does this, but were unsuccessful. In fact flipping the spins at positions $k+1$ and $k+2$ yields the state $|k+2\rangle$, but this should occur at order λ^{2s}

- But the interaction at this order contains two terms which can flip the spins:

$$(S^-_{k+1}S^+_{k+2})^{2s} \qquad (S^+_{k-1}S^-_k)^{2s}$$

- Generating the transitions:

$$|k\rangle \to |k+2\rangle \qquad |k\rangle \to |k-2\rangle$$

- Thus at this order the degenerate ground states are mixed. To find the linear combination which yields the true ground state we must diagonalize the corresponding matrix of transition amplitudes. It is of the form:

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

- Where the coefficient is calculable as:

$$\mathcal{C} = \pm 4Ks^2 \left(\frac{\lambda}{2K} \right)^{2s}$$

- The minus sign is for integer spin while the plus sign is for half odd integer spin.

- The matrix is of the circulant type, they can be easily diagonalized using the roots of unity $\quad |\frac{2\pi j}{N}\rangle = (1, \omega_j, \omega_j^2, \cdots, \omega_j^{N-1})$

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

- where $\quad \omega_j = e^{i\frac{2\pi j}{N}}$ is the $j^{\text{th}}, N^{\text{th}}$ root of unity.

- As there are only two non-zero components in the first (any) row, we get:

$$\varepsilon_j = \mathcal{C}(\omega_j^2 + \omega_j^{N-2}) = \mathcal{C}(\omega_j^2 + \omega_j^{-2})$$

$$= 2\mathcal{C}\cos\left(\frac{4\pi j}{N}\right).$$

$\mathcal{C} < 0$

$\mathcal{C} > 0$
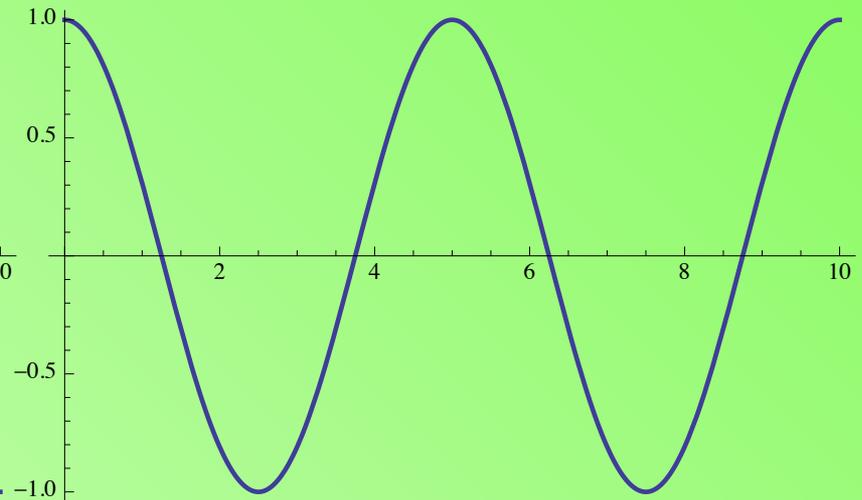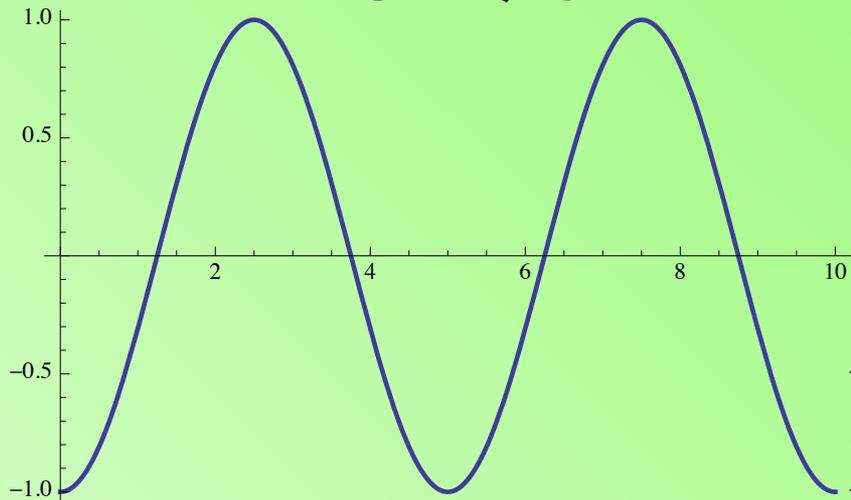
- The spectrum is symmetric about *N*/2:

$$\cos\left(\frac{4\pi([N/2]-k)}{N}\right) = \cos\left(\frac{4\pi([N/2]+k+1)}{N}\right)$$

$$k = 0, 1, 2, \cdots, [N/2]-1$$

- Except, the state at *k*=[*N*/2] is not paired.

- For integer spins $\mathcal{C} < 0$ this state is the unique ground state.

- For half-odd integer spins $\mathcal{C} > 0$ and the ground state is doubly degenerate, in accordance with Kramer's theorem.

Conclusions

- Even spin periodic chain has a non-degenerate ground state which is the symmetric or the anti-symmetric superposition of the two Néel states depending on the spin and the number of sites. The two superpositions are split in energy by $\left(\frac{\lambda}{2K}\right)^{sN}$. The excitation spectrum has a gap, proportional to 4λ and corresponding to the creation of a soliton anti-soliton pair. The spin waves are highly gapped due to the large anisotropy.

- Odd spin periodic chain has a gapless spectrum. The chain must contain at least one soliton. The chain with one up-up soliton has total spin s, while the one with a down down soliton has total spin $-s$, and these two sectors do not mix. As the position of the solitons is arbitrary, each sector is N fold degenerate. Transitions between the ground states breaks the degeneracy and form a gapless band, destroying the possibility of long range order.