Bethe ansatz for Heisenberg chain (XXZ)

N spins – N – even number

(N even or odd makes a difference!)

$s = 1/2$

Hamiltonian

$$H = \sum_{n=1}^{N} \left(J_x S_n^x S_{n+1}^x + J_y S_n^y S_{n+1}^y + S_n^z S_{n+1}^z \right)$$

$$\vec{S}_n = \frac{1}{2} \vec{\sigma}_n$$

$$\sigma_n^\alpha = I \otimes I \otimes \dots \sigma_j^\alpha \otimes I \dots \otimes I$$

in general $J_x \neq J_y \neq J_z \Rightarrow$ solution very difficult

(Baxter)

here: $J_x = J_y \neq J_z$ (XXZ)

Hamiltonian: $\longrightarrow \dfrac{H(J_x, J_z)}{J_x} - \dfrac{N\Delta}{4}$

$$\tilde{H} = \sum_{n=1}^{N} \left[\frac{1}{2} \left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+ \right) + \Delta \left(S_n^z S_{n+1}^z - \frac{1}{4} \right) \right]$$

$$\Delta = \frac{J_z}{J}$$

$-\dfrac{N\Delta}{4} \longrightarrow$ energy offset: ferromagnetic reference state has $E = 0$

periodic boundary conditions:

$$\vec{S}_{n+N} = \vec{S}_n$$

- other interesting cases:
  - twisted boundary conditions
  $$S^{\pm}_{N+1} = e^{\pm i\Phi} S^{\pm}_1$$
  - open boundary conditions

- XYZ model: most difficult but strategy similar
  - no realization as a magnetic model

- XXZ model:

  Δ distinguishes regimes

  - $\Delta > 1$: easy axis antiferromagnetic
  - $-1 < \Delta < 1$: planar regime
    - $0 < \Delta < 1$ planar antiferromagnetic
    - $-1 < \Delta < 0$ planar ferromagnetic
  - $\Delta < -1$ easy axis ferromagnetic

- other possibilities:

  XXX spin chain $(\Delta = 1)$

  XY spin chain $(\Delta = 0)$

  $\Rightarrow$ Jordan - Wigner transformation

  $\Rightarrow$ noninteracting fermion model

$\Delta \to \pm\infty$ Ising model

symmetry of spin-chain

$$\boxed{U\, H(\Delta)\, U^{-1} = -H(-\Delta)}$$

exercise/quiz

$\Rightarrow$ if we have solution to $\Delta > 0$ $\Rightarrow$ solution will be the same for $\Delta < 0$, but eigenvalue will switch sign

- symmetry: $[H, S_z] = 0$

$\rightarrow$ S_z is a good quantum number

$$H|M\rangle = E_M |M\rangle \qquad M = 1, 2, \dots$$

M - number of flipped spins

$$|M\rangle = \sum_{n_1, \dots, n_M} a(n_1, \dots, n_M)\, |n_1 \dots n_M\rangle$$

$$|n_1 \dots n_M\rangle = S^+_{n_1} \dots S^+_{n_M} |0\rangle$$

$|0\rangle = |\downarrow \dots \downarrow\rangle$ — ferromagnetic reference state

dimension of Hilbert space

$$\binom{N}{M} \qquad \sum_{M=0}^{N} \binom{N}{M} = 2^N$$

- periodic boundary conditions means

$$a(n_1, \dots, n_M) = a(n_2 \dots n_M, n_1 + N)$$

Bethe ansatz: (general)

solution of $H(\Delta)$:

$$a(n_1 \dots n_N) = \sum_{\pi} A_{\pi} \exp\left(i \sum_{j=1}^{N} k_{\pi_j} n_j\right)$$

Bethe ansatz wavefunction

sum $\sum_{\pi}$: over all permutations of k-vectors

A_{π} - phase factor associated with a particular permutation π

- to derive it:
  - solve finite difference equation associated with $H(\Delta)$
  - implement boundary conditions

- Hamiltonian can be written as a sum of two-body neighboring terms

$$H_{n,n+1} = \frac{1}{2}\left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+\right) + \Delta\left(S_n^z S_{n+1}^z - \frac{1}{4}\right)$$

recall $\quad L^{\pm}|l m\rangle = \left[l(l+1) - m(m\pm 1)\right]^{1/2} |l, m\pm 1\rangle$

$$L_z |l m\rangle = m |l m\rangle$$

$$S^{\pm} \left|\tfrac{1}{2} \mp \tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2} \pm \tfrac{1}{2}\right\rangle$$

$$S_z \left|\tfrac{1}{2}, m\right\rangle = m \left|\tfrac{1}{2}, m\right\rangle$$

(5)

$$2H_{n\,n+1}|\uparrow\rangle_n|\downarrow\rangle_{n+1} = |\downarrow\rangle_n|\uparrow\rangle_{n+1} - \Delta|\uparrow\rangle_n|\downarrow\rangle_{n+1}$$

$$2H_{n\,n+1}|\downarrow\rangle_n|\uparrow\rangle_{n+1} = |\uparrow\rangle_n|\downarrow\rangle_{n+1} - \Delta|\downarrow\rangle_n|\uparrow\rangle_{n+1}$$

$$H_{n\,n+1}|\uparrow\rangle_n|\uparrow\rangle_{n+1} = H_{n\,n+1}|\downarrow\rangle_n|\downarrow\rangle_{n+1} = 0$$

$\Downarrow$ $\Downarrow$

when using total Hamiltonian

$$2H(\Delta)|n_1\dots n_M\rangle = \sum_{\{n'\}}|n_1'\dots n_M'\rangle - N_a\Delta|n_1,\dots,n_M\rangle$$

configuration $n_1'\dots n_M'$ differs by position of one flipped spin

$$n_1' = n_1,\dots,\; n_k' = n_k \pm 1,\dots,\; n_M' = n_M$$

$\boxed{N_a - \#\text{ of anti-parallel neighboring pairs}}$

when written in first quantization, (Schrödinger equation):

$$\sum_{\{n'\}}\left[a(n_1'\dots n_M') - \Delta\, a(n_1,\dots,n_M)\right] = 2E_M\, a(n_1,\dots,n_M)$$

$\Downarrow$ $\Downarrow$

finite difference equation

- to go from second quantization to first
  - example $M=1$

$$|M\rangle = \sum_n a(n)\,|n\rangle$$

$$2H(\Delta)|M\rangle = \sum_n a(n)\,2H(\Delta)|n\rangle = 2E(\Delta)\sum_n a(n)|n\rangle$$

$$\langle n'| \rightarrow \quad \sum_n a(n)\,\langle n'|2H(\Delta)|n\rangle = 2E(\Delta)\,a(n')$$

$$\underbrace{\sum_n a(n)\left[\delta_{n',n+1} + \delta_{n',n-1} - 2\Delta\,\delta_{nn'}\right]}_{\text{Hamiltonian matrix}} = 2E(\Delta)\,a(n')$$

$$\Rightarrow a(n'+1) + a(n'-1) - 2\Delta\, a(n') = 2E(\Delta)\, a(n')$$

- interesting exercise / quiz : $M = 2$

equation for $M=1$ solved by plane-wave (magnon)

$$a(n+1) + a(n-1) - 2\Delta\, a(n) = 2E_1\, a(n)$$

$$a(n) = A e^{ikn}$$

$$E_1 = \cos k - \Delta$$

$\Rightarrow$ one flipped spin behaves like a free-particle

- $M = 2$ case: $\downarrow\downarrow\downarrow\overset{n_1}{\uparrow}\downarrow\downarrow \dots \downarrow\overset{n_2}{\uparrow}\downarrow \dots$

$\Rightarrow a(n_1, n_2)$

distinguish two cases:

- flipped spins <u>are not</u> neighbors

  $n_2 > n_1 + 1$

- flipped spins <u>are</u> neighbors

  $n_2 = n_1 + 1$

First case:

finite difference equation

$$a(n_1-1,n_2)+a(n_1+1,n_2)+a(n_1,n_2-1)+a(n_1,n_2+1)$$
$$-4\Delta a(n_1,n_2) = 2E_2\, a(n_1,n_2)$$

solution: $a(n_1,n_2) = A_{12}\, e^{i(k_1 n_1 + k_2 n_2)} + A_{21}\, e^{i(k_2 n_1 + k_1 n_2)}$

substituting results in eigenvalue

$$E_2 = \cos k_1 - \Delta + \cos k_2 - \Delta$$

---

substitution:

$$A_{12}\, e^{i(k_1 n_1 + k_2 n_2)}\left[e^{-ik_1} + e^{ik_1} + e^{-ik_2} + e^{ik_2} - 4\Delta\right]$$
$$+ A_{21}\, e^{i(k_2 n_1 + k_1 n_2)}\left[e^{-ik_2} + e^{ik_2} + e^{-ik_1} + e^{ik_1} - 4\Delta\right]$$
$$= 2E_2\left[A_{12}\, e^{ik_1 n_1 + k_2 n_2} + A_{21}\, e^{ik_2 n_1 + k_1 n_2}\right]$$

true for arbitrary coefficients if

$$E_2 = \cos k_1 - \Delta + \cos k_2 - \Delta$$

$\Rightarrow$ two "free particles"

BUT!!!

- two flipped spins can also come together!
  - must consider case 2 ($n_2 = n_1 + 1$) and make it consistent with case 1

case 2: $n_2 = n_1 + 1$ $\quad \downarrow\downarrow\downarrow \overset{n_1}{\uparrow}\overset{n_2}{\uparrow}\downarrow\downarrow$

- clearly: Hamiltonian <u>can not</u> flip n_1 to n_2 and vice versa

- finite difference equation

$$a(n_1-1, n_2) + a(n_1, n_2+1) - 2\Delta\, a(n_1, n_2) = 2E\, a(n_1, n_2)$$

- to make it consistent with case 1 we write the finite difference equation from case 1 ~~$n_2 = n_1+1$~~ for $n_2 = n_1 + 1$

$$a(n_1-1, n_1+1) + a(n_1+1, n_1+1) + a(n_1, n_1) + a(n_1, n_1+2) - 4\Delta\, a(n_1, n_1+1) = 2E\, a(n_1, n_1+1)$$

for case 2 we have with $n_2 = n_1+1$

$$a(n_1-1, n_1+1) + a(n_1, n_1+2) - 2\Delta\, a(n_1, n_1+1) = 2E\, a(n_1, n_1+1)$$

subtract case 2 from case 1

$$\boxed{a(n_1, n_1) + a(n_1+1, n_1+1) - 2\Delta\, a(n_1, n_1+1) = 0}$$

- substitute form of wavefunction

$$(A_{12}+A_{21})\left[1+e^{i(k_1+k_2)}\right] - 2\Delta A_{12}\, e^{ik_2} - 2\Delta A_{21}\, e^{ik_1} = 0$$

$$\Downarrow$$

$$\frac{A_{21}}{A_{12}} = -\frac{e^{i(k_1+k_2)} - 2\Delta e^{ik_2} + 1}{e^{i(k_1+k_2)} - 2\Delta e^{ik_1} + 1}$$

$$= -\frac{e^{i\frac{k_1+k_2}{2}} - 2\Delta e^{i\frac{k_2-k_1}{2}} + e^{-i\frac{k_1+k_2}{2}}}{e^{i\frac{k_1+k_2}{2}} - 2\Delta e^{i\frac{k_1-k_2}{2}} + e^{-i\frac{k_1+k_2}{2}}} \Rightarrow \left|\frac{A_{21}}{A_{12}}\right| = 1$$

$$= -\frac{2\cos\left(\frac{k_1+k_2}{2}\right) - 2\Delta\cos\left(\frac{k_1-k_2}{2}\right) - 2\Delta i\sin\left(\frac{k_1-k_2}{2}\right)}{2\cos\left(\frac{k_1+k_2}{2}\right) - 2\Delta\cos\left(\frac{k_1-k_2}{2}\right) + 2\Delta i\sin\left(\frac{k_1-k_2}{2}\right)}$$

$$\frac{A_{21}}{A_{12}} = e^{-i\Theta(k_1,k_2)} \qquad \left(\text{since } \left|\frac{A_{21}}{A_{12}}\right| = 1\right)$$

$$\cancel{\frac{A_{21}}{A_{12}}} = e^{-i\Theta(k_1,k_2)} = -\frac{\cancel{2}\left[\cos\left(\frac{k_1+k_2}{2}\right) - \Delta\cos\left(\frac{k_1-k_2}{2}\right) - i\Delta\sin\left(\frac{k_1-k_2}{2}\right)\right]}{\cos\left(\frac{k_1+k_2}{2}\right) - \Delta\cos\left(\frac{k_1-k_2}{2}\right) + i\Delta\sin\left(\frac{k_1-k_2}{2}\right)}$$

$$\Downarrow$$

$$\boxed{\Theta(k_1,k_2) = 2\cot^{-1}\left[\frac{\Delta\sin\left(\frac{k_1-k_2}{2}\right)}{\cos\left(\frac{k_1+k_2}{2}\right) - \Delta\cos\left(\frac{k_1-k_2}{2}\right)}\right]}$$

- two particles which interact via a "scattering process" described by phase $\Theta(k_1,k_2)$

- general solution for $M = 2$

$$a(n_1, n_2) = A_{12}\left[e^{ik_1 n_1 + k_2 n_2} + e^{i\frac{\Theta(k_1,k_2)}{2}} e^{i(k_2 n_1 + k_1 n_2)}\right]$$

- "complete" picture emerges when one considers

$M = 3$

$a(n_1, n_2, n_3) \rightarrow$ $\downarrow\downarrow\uparrow\downarrow\downarrow \dots \uparrow - \uparrow\downarrow\downarrow$

possible cases:

1.) $n_1 + 1 < n_2$ $\quad n_2 + 1 \leq n_3$ (all three separate)

$\downarrow\uparrow\downarrow \dots \uparrow \dots \uparrow \dots$

2.) $n_1 + 1 = n_2$ $\quad n_2 + 1 < n_3$ (n_1, n_2 neighbors n_3 separate)

$\downarrow\uparrow\downarrow \dots \downarrow\uparrow\uparrow\downarrow \dots$

3.) $n_1 < n_2 + 1$ $\quad n_2 + 1 = n_3$ (n_2, n_3 neighbors n_1 separate)

$\dots \downarrow\uparrow\uparrow\downarrow \dots \downarrow\uparrow\downarrow \dots$

4.) $n_1 + 1 = n_2$ $\quad n_2 + 1 = n_3$

$\dots \downarrow\uparrow\uparrow\uparrow\downarrow \dots$

case 1:

$$a(n_1-1, n_2, n_3) + a(n_1+1, n_2, n_3)$$
$$+ a(n_1, n_2-1, n_3) + a(n_1, n_2+1, n_3)$$
$$+ a(n_1, n_2, n_3-1) + a(n_1, n_2, n_3+1)$$
$$- 6\Delta a(n_1, n_1, n_3) = 2E_3 a(n_1, n_2, n_3)$$

assume form of wavefunction:

$$a(n_1, n_2, n_3) = A_{123} e^{i(k_1 n_1 + k_2 n_2 + k_3 n_3)} + A_{132} e^{i(k_1 n_1 + k_3 n_2 + k_2 n_3)}$$
$$+ A_{213} e^{i(k_2 n_1 + k_1 n_2 + k_3 n_3)} + A_{231} e^{i(k_2 n_1 + k_3 n_2 + k_1 n_3)}$$
$$+ A_{312} e^{i(k_3 n_1 + k_1 n_2 + k_2 n_3)} + A_{321} e^{i(k_3 n_1 + k_2 n_2 + k_1 n_3)}$$

substitution into Schrödinger equation results in:

$$E_3 = \cos k_1 - \Delta + \cos k_2 - \Delta + \cos k_3 - \Delta$$

case 2

$$n_1+1=n_2 \qquad n_3>n_2+1$$

$$a(n_1-1,\ n_1+1,\ n_3)+a(n_1,\ n_1+2,\ n_3)$$
$$+\,a(n_1,\ n_1+1,\ n_3-1)+a(n_1,\ n_1+1,\ n_3+1)$$
$$-\,4\Delta\, a(n_1,\ n_1+1,\ n_3)=2E_3\, a(n_1,n_1+1,n_3)$$

writing the Schrödinger equation for case 1

with $n_1+l_1=n_2$ we have

$$a(n_1-1,\ n_1+1,\ n_3)+a(n_1+1,\ n_1+1,\ n_3)$$
$$+\,a(n_1,\ n_1,\ n_3)+a(n_1,\ n_1+2,\ n_3)$$
$$+\,a(n_1,\ n_1+1,\ n_3-1)+a(n_1,\ n_1+1,\ n_3+1)$$
$$-\,6\Delta\, a(n_1,\ n_1+1,\ n_3)=2E_3\, a(n_1,n_1+1,n_3)$$

again subtract one from the other:

$$a(n_1,\ n_1,\ n_3)+a(n_1+1,\ n_1+1,\ n_3)-2\Delta a(n_1,\ n_1+1,\ n_3)=0$$
$$\cancel{=2E_3\, a(n_1,n_1+1,n_3)}$$

notice! if n_3 was not there this would be the same equation as what we obtained for the $N=2$ case:

$$a(n_1,\ n_1)+a(n_1+1,\ n_1+1)-2\Delta a(n_1,n_1+1)=0$$

it leads to: $A_{123}=A_{213}\, e^{i\frac{\Theta}{2}(k_1,k_2)}$

$\Theta(k_1,k_2)\longrightarrow$ same phase case 3

make long story short: $n_1 < n_2 - 1$ $\quad n_2 + 1 = n_3$

$$a(n_1, n_2, n_2) + a(n_1, n_2+1, n_2+1) - 2\Delta(n_1, n_2, n_2+1) = 0$$

$$\Downarrow$$

$$A_{123} = A_{132}\, e^{\frac{i\Theta(k_2, k_3)}{2}}$$

$$\Downarrow \qquad \Downarrow$$

One can reach any permutation

$$A_{123} \to A_{213} \to A_{231}$$

case 4

$\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow$ $\quad n_1 + 1 = n_2$ $\quad n_2 + 1 = n_3$

can obtain several equivalent conditions

$$a(n_1, n_1+1, n_1+1) + a(n_1, n_1+2, n_1+2)$$
$$- 2\Delta\, a(n_1, n_1+1, n_1+2) = 0$$

- restatement of previous findings

$$\Downarrow \qquad \Downarrow$$

$A_{123} \to$ factorises into $A_{12}\; A_{13}\; A_{23}$

for M flipped spins:

$$A_\pi = N \exp\left[\frac{i}{2} \sum_{i<j} \Theta(k_{\pi_i}, k_{\pi_j})\right]$$

eigenvalue: $\quad E_M = \sum_{i=1}^{M} (\cos k_i - \Delta)$

- so far: Bethe ansatz wavefunction derived
  - phases represent scattering processes, but the particles are "otherwise independent"

- to complete formalism ⇒ one more element
  - boundary conditions
  - periodic boundary conditions:
    - case $M = 1$

$$a(n) = a(n+N)$$

$$a(n) = A e^{ikn} = A e^{ikn} e^{ikN}$$

$$kN = \lambda 2\pi$$

$$k = \frac{2\pi\lambda}{N}$$

$$\lambda = 0, 1, \dots, N-1$$

- familiar result for particle on lattice with PBC

- case $M = 2$

$$a(n_1, n_2) = a(n_2, n_1 + N)$$

using form of wavefunction:

$$A_{12}\, e^{i(k_1 n_1 + k_2 n_2)} + A_{21}\, e^{i(k_2 n_1 + k_1 n_2)}$$

$$= A_{12}\, e^{i(k_1 n_2 + k_2 n_1)} e^{ik_2 N} + A_{21}\, e^{i(k_2 n_2 + k_1 n_1)} e^{ik_1 N}$$

$$\longrightarrow \quad A_{12} = A_{21}\, e^{ik_1 N} \;/\; A_{21} = A_{12}\, e^{ik_2 N}$$

$$\frac{A_{12}}{A_{21}} e^{-ik_1 N} = 1 \Rightarrow \qquad k_1 N = 2\pi\lambda_1 + \Theta(k_1, k_2)$$

$$\frac{A_{21}}{A_{12}} e^{-ik_2 N} = 1 \Rightarrow \qquad k_2 N = 2\pi\lambda_2 + \Theta(k_2, k_1)$$

$$(k_1 + k_2) N = 2\pi(\lambda_1 + \lambda_2)$$

total momentum of two-particle system

case $M = 3$

$$a(n_1, n_2, n_3) = a(n_2, n_3, n_1 + N)$$

$$A_{123} e^{i(k_1 n_1 + k_2 n_2 + k_3 n_3)} + A_{132} e^{i(k_1 n_1 + k_3 n_2 + k_2 n_3)}$$
$$+ A_{213} e^{i(k_2 n_1 + k_1 n_2 + k_3 n_3)} + A_{231} e^{i(k_2 n_1 + k_3 n_2 + k_1 n_3)}$$
$$+ A_{312} e^{i(k_3 n_1 + k_1 n_2 + k_2 n_3)} + A_{321} e^{i(k_3 n_1 + k_2 n_2 + k_1 n_3)}$$

$$= A_{123} e^{i(k_1 n_2 + k_2 n_3 + k_3 n_1)} e^{ik_3 N} + A_{132} e^{i(k_1 n_2 + k_3 n_3 + k_2 n_1)} e^{ik_2 N}$$
$$+ A_{213} e^{i(k_2 n_2 + k_1 n_3 + k_3 n_1)} e^{ik_3 N} + A_{231} e^{i(k_2 n_2 + k_3 n_3 + k_1 n_1)} e^{ik_1 N}$$
$$+ A_{312} e^{i(k_3 n_2 + k_1 n_3 + k_2 n_1)} e^{ik_2 N} + A_{321} e^{i(k_3 n_2 + k_2 n_3 + k_1 n_1)} e^{ik_1 N}$$

for example the terms A_{123} with $e^{i(k_1 n_1 + k_2 n_2 + k_3 n_3)}$

are

$$A_{123} = A_{231}\, e^{i k_1 N}$$

other terms with equivalent plane-wave factors

$$\Rightarrow \quad A_{132} = A_{321}\, e^{i k_1 N}$$

$$A_{213} = A_{132}\, e^{i k_2 N}$$

$$A_{231} = A_{312}\, e^{i k_2 N}$$

$$A_{312} = A_{123}\, e^{i k_3 N}$$

$$A_{321} = A_{213}\, e^{i k_3 N}$$

$A_{312} \to A_{321}$

$A_{123} \to A_{213}$

only three are different

resulting equations: <u>Bethe ansatz equations</u>

$$k_j N = 2\pi \lambda_j + \sum_{i=1,\, i\neq j}^{M} \Theta(k_i, k_j) \qquad [\text{for general } M]$$

---

numerical strategy to solve Bethe

- choose λ_j
- choose initial k-vectors

  (for example: corresponding Fermi sea)
- solve self-consistently

- Bethe ansatz equations are algebraic equations for a combinatorial problem

  (M-equations, even though Hilbert space is $\binom{N}{M}$ dimensional)

Summary:

- spin-$\frac{1}{2}$ anisotropic Heisenberg model (XXZ) can be solved using the Bethe ansatz wave function
- the Bethe ansatz wavefunction consists of a sum of products of plane-waves. In each term in the sum, k vectors are permuted.
- the phase of each term in the sum can be factorized into two-particle scattering processes → phase determined by interaction parameter
- periodic boundary conditions result in M equations for the momentum vectors $\underline{k}$ in terms of phases & quantum numbers λ
- much better than the original Hilbert space, which is $\binom{N}{M}$ dimensional
- algebraic equations can be solved analytically in the thermodynamic limit
- they can be solved numerically as well
- ground state and excited state properties are accessible
- finite T properties are accessible