

XY Model revisited

Manuela Carvalho de Almeida

Instituto de Física, Universidade de Brasília

September 4, 2014

A simple case: 2 sites

- Let us consider a simple system of two qubits with the XY type interaction¹. The Hamiltonian is

$$H(h, \gamma) = -\frac{(1 + \gamma)}{2} \sigma_1^x \sigma_2^x - \frac{(1 - \gamma)}{2} \sigma_1^y \sigma_2^y - \frac{h}{2} (\sigma_1^z + \sigma_2^z). \quad (1)$$

- γ - anisotropy factor
- h - external magnetic field in the z direction.
- σ_i^α - Pauli matrices of the i -th qubit, with $\alpha = x, y, z$.
- Simple example of the general XY model, for N qubits

$$H = -\sum_{i=1}^N \left[\left(\frac{1 + \gamma}{2} \right) \sigma_i^x \sigma_{i+1}^x + \left(\frac{1 - \gamma}{2} \right) \sigma_i^y \sigma_{i+1}^y + h \sigma_i^z \right], \quad (2)$$

¹2009, Oh Physics Letters A 373 (2009) 644-647

In the matrix form, we have

$$H(h, \gamma) = - \begin{pmatrix} h & 0 & 0 & \gamma \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ \gamma & 0 & 0 & -h \end{pmatrix} = H_{\text{even}} + H_{\text{odd}} \quad (3)$$

The basis chosen is

$|00\rangle, |01\rangle = \sigma_2^+ |00\rangle, |10\rangle = \sigma_1^+ |00\rangle, |11\rangle = \sigma_1^+ \sigma_2^+ |00\rangle$, where

- 0 means empty,
- 1 means occupied.

$$H_{\text{even}} = \begin{pmatrix} h & \gamma \\ \gamma & -h \end{pmatrix} \quad (4)$$

- Subspace spanned by $|00\rangle, |11\rangle$
- Eigenstates

$$E_{\pm}^{\theta} = \pm \sqrt{\gamma^2 + h^2} \quad (5)$$

$$|E_{-}^{\theta}\rangle = \cos \frac{\theta}{2} |00\rangle + \sin \frac{\theta}{2} |11\rangle \quad (6)$$

$$|E_{+}^{\theta}\rangle = -\sin \frac{\theta}{2} |00\rangle + \cos \frac{\theta}{2} |11\rangle \quad (7)$$

where $\tan \theta = \gamma/h$

$$H_{\text{odd}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (8)$$

- Subspace spanned by $|01\rangle, |10\rangle$
- Eigenstates

$$E_{\pm}^0 = \pm 1 \quad (9)$$

$$|E_{\pm}^0\rangle = \frac{1}{\sqrt{2}}(|01\rangle \mp |10\rangle) \quad (10)$$

Level Crossing

Note that when $\gamma^2 + h^2 = 1$, there is a level crossing

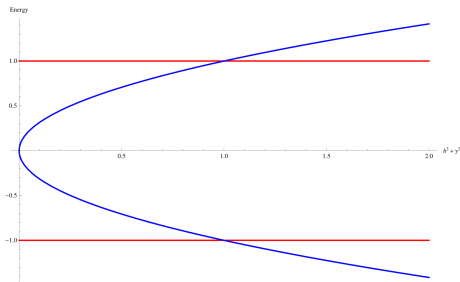


Figure : Level-crossing

- 1 What happens if we generalize to N sites, is there still a level crossing?
- 2 Which observables can measure this level crossing?²

²A. P. Balachandran, T. R. Govindarajan, Amilcar R. de Queiroz, A. F. Reyes-Lega, PRL110,080503 (2013)

Looking at XY model

- Spin chain with N sites.
- a : distance between the sites.
- $L = Na$: length of the chain.
- Periodic boundary conditions: $N + j \equiv j$, where $j = 1, \dots, N$ are the label of the sites.

Writing again the Hamiltonian³

$$H(h, \gamma) = -\frac{1}{2} \sum_{j=1}^N \left[\left(\frac{1+\gamma}{2} \right) \sigma_j^x \sigma_{j+1}^x + \left(\frac{1-\gamma}{2} \right) \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right].$$

³F. Franchini, *Notes on Bethe Ansatz Techniques*, Trieste, Italy, 2011.

Phase Diagram

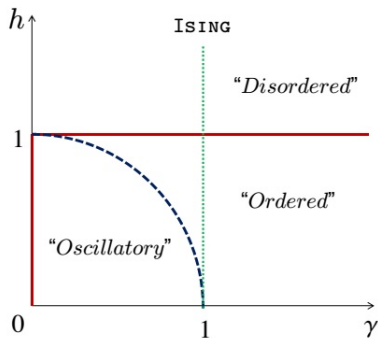


Figure : Phase diagram for ferromagnetic XY spin chain⁴

- $\gamma = 0$ - XX model,
- $\gamma = 1$ - Ising model.

⁴F. Franchini, *Notes on Bethe Ansatz Techniques*, Trieste, Italy, 2011.

Second quantization picture

After a Jordan-Wigner transformation, we arrive to a second quantized version of the XY Hamiltonian

$$H_{bulk} = \frac{-1}{2} \sum_{j=1}^{N-1} \left(\psi_j^\dagger \psi_{j+1} + \psi_{j+1}^\dagger \psi_j + \gamma (\psi_j^\dagger \psi_{j+1}^\dagger + \psi_{j+1} \psi_j) - 2h \psi_j^\dagger \psi_j \right) - \frac{hN}{2} \quad (11)$$

$$H_{boundary} = \frac{T_N}{2} (\psi_N^\dagger \psi_1 + \psi_1^\dagger \psi_N + \gamma (\psi_N^\dagger \psi_1^\dagger + \psi_1 \psi_N) - 2h \psi_N^\dagger \psi_N) \quad (12)$$

where

$$T_N = \prod_{i=1}^N \sigma_i^z \quad (13)$$

The T_N operator and boundary conditions

- From Jordan-Wigner, one can see there is a relation between spin in z-direction and number of fermions.

$$\sigma^z = 1 - 2\psi^\dagger\psi \quad (14)$$

- For $\gamma \neq 0 \rightarrow [H, \sigma^z] \neq 0$ - Number of fermions is not conserved.
- Since fermions are created in pair, the 'parity' of number of fermions is conserved.
- T_N is the operator that counts such parity

$$T_N = (-1)^{Q_N}, \quad Q_N = \sum_{i=1}^N \psi_i^\dagger \psi_i \equiv \text{Number of fermions} \quad (15)$$

- $T_N = +1$ if Q_N even, $T_N = -1$ if Q_N odd

- The sign of the boundary term of the Hamiltonian (??) varies depending on the number of fermions.
- In order to correct the sign of the Hamiltonian, we have to impose different boundary conditions for each sector
- For the even sector

$$\psi_{j+N} = -\psi_j \quad (16)$$

- For the odd sector

$$\psi_{j+N} = \psi_j \quad (17)$$

- Since $T_N^2 = 1$, one can build up a projector and separate the theory in two sectors.

$$H = \frac{1 + T_N}{2} H_{\text{even}} + \frac{1 - T_N}{2} H_{\text{odd}}. \quad (18)$$

- H_{even} is H with antiperiodic boundary conditions.
- H_{odd} is H with periodic boundary conditions.

Diagonalizing the Hamiltonian

One can write ψ e ψ^\dagger in normal modes using the discrete Fourier transform and applying the correct boundary conditions to each sector

$$\psi_j = \frac{1}{\sqrt{aN}} \sum_n e^{ik_nja} b_{k_n}, \quad (19)$$

$$-\frac{N-1}{2} \leq n \leq \frac{N-1}{2}$$

$$\psi_j^\dagger = \frac{1}{\sqrt{aN}} \sum_n e^{-ik_nja} b_{k_n}^\dagger. \quad (20)$$

where

$$k_n = \frac{2\pi}{L} \left(n + \frac{P}{2} \right), \quad (21)$$

and

$P = 1$, antiperiodic boundary conditions,

$P = 0$, periodic boundary conditions.

The inverse transformation is

$$b_n \equiv b_{k_n} = \sqrt{\frac{a}{N}} \sum_{j=1}^N e^{-ik_nja} \psi_j, \quad (22)$$

$$b_n^\dagger \equiv b_{k_n}^\dagger = \sqrt{\frac{a}{N}} \sum_{j=1}^N e^{ik_nja} \psi_j^\dagger. \quad (23)$$

The anticommutation relations for b

$$\{b_n, b_m\} = \{b_n^\dagger, b_m^\dagger\} = 0, \quad (24)$$

$$\{b_n, b_m^\dagger\} = a \delta_{n,m}. \quad (25)$$

Defining

- $b_{-n} \equiv d_n^\dagger$: creates an antiparticle with momentum k_n .
- $b_{-n}^\dagger \equiv d_n$: destroys an antiparticle with momentum k_n .

$$\begin{aligned}
 H = & -\frac{hN}{2} \\
 & -\frac{1}{2a} \left[(\cos(k_0 a) - h)(b_{k_0}^\dagger b_{k_0} + d_{k_0}^\dagger d_{k_0}) + i\gamma \sin(k_0 a)(b_{k_0}^\dagger d_{k_0} + b_{k_0} d_{k_0}^\dagger) \right] \\
 & -\frac{1}{a} \sum_{n=1}^{\frac{(N-1)}{2}} \left[(\cos(k_n a) - h)(b_n^\dagger b_n + d_n d_n^\dagger) + i\gamma \sin(k_n a)(b_n^\dagger d_n + b_n d_n^\dagger) \right]
 \end{aligned}$$

- The hamiltoninan has three important terms

$$H = \mu N + H_{k_0} + \tilde{H}. \quad (26)$$

- $\mu N \equiv -hN/2$ is a chemical potential.
- The H_{k_0} is a special case. For periodic boundary conditions it represents a zero mode. ($k_0 = 0$)

Diagonalizing - Bogoliubov transformation

- Because $\gamma \neq 0$ there is a term mixing b 's e d 's operators.
- Need to introduce new operators that are linear combination of b 's and d 's \implies Bogoliubov transformation.
- It takes Ψ_n to $\Phi_n^\dagger \equiv (\chi_n^\dagger \eta_n^\dagger)$, eigenvectors of \mathcal{H}_n .

$$\begin{pmatrix} b_n \\ d_n \end{pmatrix} = \begin{pmatrix} \cos \nu_n & \sin \nu_n \\ -\sin \nu_n & \cos \nu_n \end{pmatrix} \begin{pmatrix} \chi_n \\ \eta_n \end{pmatrix}, \quad (27)$$

with ν_n given by

$$\tan 2\nu_n = \frac{\sin(k_n a)}{h - \cos(k_n a)}. \quad (28)$$

- The Hamiltonian now becomes

$$\tilde{H} = -\frac{1}{a} \sum_{n=1}^{\frac{(N-1)}{2}} \Psi_n^\dagger \mathcal{H}_n \Psi_n, \quad \Psi_n^\dagger = \begin{pmatrix} b_n^\dagger & d_n^\dagger \end{pmatrix}$$
$$\mathcal{H}_n = \begin{pmatrix} \cos(k_n a) - h & i\gamma \sin(k_n a) \\ -i\gamma \sin(k_n a) & -(\cos(k_n a) - h) \end{pmatrix}. \quad (29)$$

- The eigenvalue of \mathcal{H}_n are

$$\epsilon(k_n) = \sqrt{(h - \cos(k_n a))^2 + \gamma^2 \sin^2(k_n a)} \quad (30)$$

- The hamiltonian

$$H^+ = \frac{\epsilon(k_0)}{2a} (\chi_{k_0}^\dagger \chi_{k_0} + \eta_{k_0} \eta_{k_0}^\dagger) + \frac{1}{a} \sum_{n=1}^{\frac{N-1}{2}} \epsilon(k_n) \left\{ \chi_n^\dagger \chi_n + \eta_n \eta_n^\dagger \right\}, \quad (31)$$

with $P = 1$ in k_n .

- *There is no zero mode.*
- Indeed, χ_n^\dagger creates a *quasiparticle* state.
- The ground state is

$$\chi_n |GS\rangle_+ = 0 \quad \eta_n^\dagger |GS\rangle_+ = 0, \quad n = 0, \dots, (N-1)/2. \quad (32)$$

$k_0 = 0$: odd sector

- The hamiltonian

$$H^- = -\frac{1}{a}(1-h)b_0^\dagger b_0 - \frac{1}{a} \sum_{n=1}^{\frac{(N-1)}{2}} \epsilon(k_n) \left\{ \chi_n^\dagger \chi_n + \eta_n \eta_n^\dagger \right\}, \quad (33)$$

with $P = 0$ in k_n .

- *There is* a zero mode!

$$k_0 = \frac{2\pi \cdot 0}{L} = 0. \quad (34)$$

- The rotation angle in the Bogoliubov transformation

$$\tan 2\nu_n = \frac{\sin k_n a}{h - \cos k_n a}, \quad (35)$$

is zero, because $n = 0$ implies $\nu_0 = 0 \Rightarrow$ the zero mode is *invariant* under Bogoliubov transformation,

$$\chi_0 = b_0. \quad (36)$$

The zero mode energy term implies two regimes:

- ① When $h < 1$, weak external field

$$-(1 - h) = \epsilon(0) \Rightarrow \text{sign } \epsilon(0) = \text{sign } \epsilon(k_n), \quad (37)$$

$$H^- = \frac{1}{a} \epsilon(0) \chi_0^\dagger \chi_0 + \frac{1}{a} \sum_{n=1}^{(N-1)/2} \epsilon(k_n) \left\{ \chi_n^\dagger \chi_n + \eta_n \eta_n^\dagger \right\}, \quad (38)$$

- ② When $h > 1$, strong external field

$$-(1 - h) = -\epsilon(0) \Rightarrow \text{sign } \epsilon(0) = -\text{sign } \epsilon(k_n), \quad (39)$$

$$H^- = -\frac{1}{a} \epsilon(0) \chi_0^\dagger \chi_0 + \frac{1}{a} \sum_{n=1}^{(N-1)/2} \epsilon(k_n) \left\{ \chi_n^\dagger \chi_n + \eta_n \eta_n^\dagger \right\}. \quad (40)$$

- The ground state should be the one which

$$\chi_n |GS'\rangle_- = 0 \quad \eta_n^\dagger |GS'\rangle_- = 0, \quad n = 1, \dots, (N-1)/2, \quad (41)$$

but this state is forbidden by the constrain in the sector: the number of excitations must be odd!

- The true ground state of this sector is

$$|GS\rangle_- = \chi_0^\dagger |GS'\rangle_- = b_0^\dagger |GS'\rangle_-. \quad (42)$$

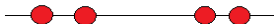


Figure : Particles created from $|GS\rangle$: Even sector

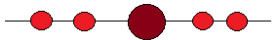


Figure : Particles created from $\chi_0^\dagger |GS\rangle$: Odd sector

Ground state energy in the thermodynamic limit

- The ground state energy of the even sector is

$$E_0^+ = \sum_{n=0}^{(N-1)/2} \epsilon \left[\frac{2\pi}{N} \left(n + \frac{1}{2} \right) \right] \quad (43)$$

- The ground state energy of the odd sector for $h < 1$ is

$$E_0^- = -(1-h) + \sum_{n=0}^{(N-1)/2} \epsilon(k_n) = \sum_{n=0}^{(N-1)/2} \epsilon \left(\frac{2\pi n}{N} \right) \quad (44)$$

- The difference between ground state energies is

$$E_0^+ - E_0^- = O \left(\frac{1}{N} \right) \rightarrow 0, \quad N \rightarrow \infty. \quad (45)$$

- $E_0^+ = E_0^-$, for $h < 1$, in the thermodynamic limit.
- The spectrum is degenerate for $h < 1$, but this degeneracy has a thermodynamic origin.

Ground state energy plotted

There is a level crossing!

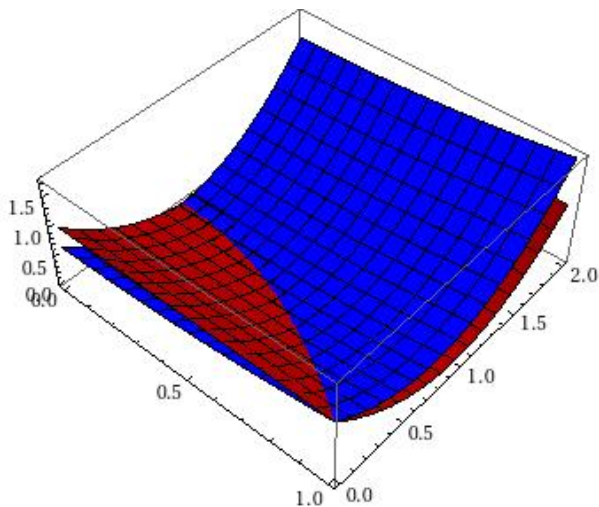


Figure 2: 3d plot of energy $E_0(x, y)$

Ground state energy plotted

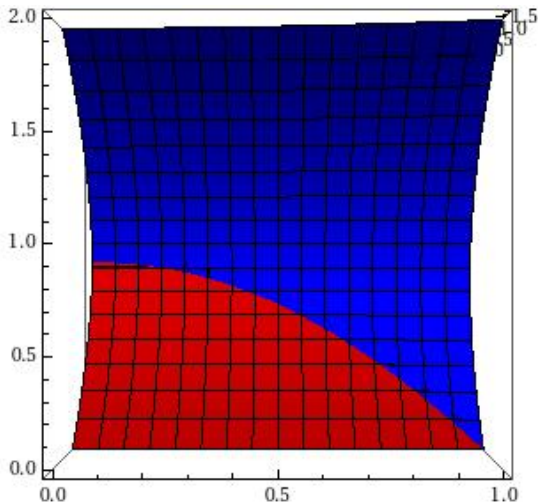


Figure : 3d plot of energy $\times h \times \gamma$

Ground state energy plotted

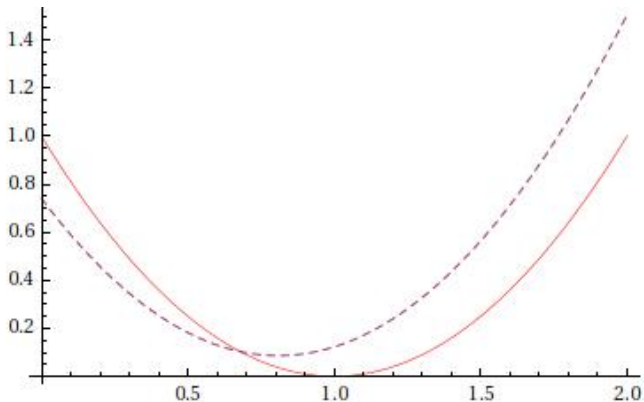


Figure : Energy versus h

Others boundary conditions

Now, let's analyze other possible boundary conditions. One can choose, for each sector

$$\psi_{j+N} = \pm e^{i\theta} \psi_j, \quad (46)$$

a quasiperiodic boundary condition. Using Bloch's theorem, ψ_j can be written as

$$\psi_j = e^{i\theta j/N} \phi_j, \quad (47)$$

where $\phi_{j+N} = \pm \phi_j$, depending on the sector. Indeed,

$$\psi_j = e^{i\theta(j+N)/N} \phi_{j+N} = \pm e^{i\theta} (e^{i\theta j/N} \phi_j) = \pm e^{i\theta} \psi_j \quad (48)$$

We can substitute the operators ϕ_i on the fermionic Hamiltonian, and get

$$\begin{aligned} H &= -\frac{1}{2} \sum_{j=1}^N \left[\left(e^{i\theta/N} \phi_j^\dagger \phi_{j+1} + e^{-i\theta/N} \phi_{j+1}^\dagger \phi_j \right) \right. \\ &\quad \left. + \gamma \left(e^{-i(2j+1)\theta/N} \phi_j^\dagger \phi_{j+1}^\dagger + e^{i(2j+1)\theta/N} \phi_{j+1} \phi_j \right) - 2h \phi_j^\dagger \phi_j \right] \\ &= H_\theta \end{aligned} \tag{49}$$

Note that we still have $[T_N, H_\theta] = 0$, therefore the equivalence below is valid

$$(H_0, bc_\theta) \Leftrightarrow (H_\theta, bc_0). \tag{50}$$

The ϕ operators obey a fermionic anticommutation relation.

Doing all the calculations done before, we see this 'quasiperiodic' boundary conditions leads to a redefinitions of the energy eigenvalues

$$\epsilon(\tilde{k}_n) = \sqrt{(h - \cos(k_n a + \theta/N))^2 + \gamma^2 \sin^2(k_n a + \theta/N)} \quad (51)$$

and of the Bogoliubov's angle

$$\tan 2\tilde{\nu}_n = \frac{\sin(k_n a + \theta/N)}{h - \cos(k_n a + \theta/N)}. \quad (52)$$

θ has the role of a flux in the chain and it can be tunned to measure the zero mode on the lab!

A more general case is to consider the boundary condition $\psi_{j+N} = e^{i\theta Q_N} \psi_j$, which will lead to the following dressed operators

$$\psi_j = e^{i\theta Q_{j-1}} \phi_j, \quad \psi_j^\dagger = e^{i\theta Q_{j-1}} \phi_j^\dagger. \quad (53)$$

Now, the anticommutation relations become different for ϕ_j, ϕ_j^\dagger

$$\phi_j^\dagger \phi_k + e^{i\epsilon\theta(N_j-1)} \phi_k \phi_j^\dagger = \delta_{jk} \quad (54)$$

$$\phi_j^\dagger \phi_k^\dagger + e^{i\epsilon\theta(N_j-1)} \phi_k^\dagger \phi_j^\dagger = \phi_j \phi_k + e^{i\epsilon\theta(N_j-1)} \phi_k \phi_j = 0 \quad (55)$$

$$\epsilon = \begin{cases} 1, & k > j \\ -1, & k < j \\ 0, & k = j \end{cases} \quad (56)$$

Now, the operators ϕ_i satisfy an "anyonic" anticommutation relation⁵.

⁵M. D. Girardeau, PRL97,100402 (2006)

The anyonic Hamiltonian then is

$$\begin{aligned} H &= -\frac{1}{2} \sum_{j=1}^N \left[\left(\phi_j^\dagger \phi_{j+1} e^{i\theta N_j} + e^{-i\theta N_j} \phi_{j+1}^\dagger \phi_j \right) \right. \\ &\quad \left. + \gamma \left(e^{-2i\theta Q_{j-1}} \phi_j^\dagger \phi_{j+1}^\dagger e^{i\theta N_j} + e^{2i\theta Q_{j-1}} e^{-i\theta N_j} \phi_{j+1} \phi_j \right) - 2h \phi_j^\dagger \phi_j \right] \\ &= H_\theta \end{aligned} \tag{57}$$

- See these aspects in the point of view of correlation functions.
- We can play with different boundary conditions.
- Continuum limit: which is the QFT regularized by the XY model?⁶

⁶Manuel Asorey, Fernando Falceto, Germán Sierra, Nuclear Physics B 622 [FS] (2002) 593-614