

## \* ONE-DIMENSIONAL SPIN MODELS

- We have seen that one may construct different types of spin models with an optical lattice of XXZ and bilinear-biquadratic (with spin-1 systems). We may also control the lattice geometry to a large extent, introducing g. frustration. Now, it's time to see some of these models "in action".

In this lecture we will have a look briefly to some interesting one-dimensional spin models, introducing important concepts in our way. We will see that even apparently simple models may have a rich and very nontrivial physics!

### \* SPIN- $\frac{1}{2}$ XXZ CHAIN

- As mentioned in previous lectures, the XXZ spin- $\frac{1}{2}$  chain may be implemented in optical lattices using polar lattice gases (p. 66) or super-exclusion (p. 67):

$$\hat{H} = J \sum_n \left[ (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + \Delta S_n^z S_{n+1}^z \right]$$

Note: in a superlattice lattice ABAB... we may introduce  $S_i^{\pm} \rightarrow (-1)^i S_i^y, S_i^z \rightarrow S_i^z$  which keeps commutation rules and changes  $J_{x,y} \rightarrow -J_{x,y}, J_z \rightarrow J_z$ . We may hence choose  $J > 0$  without loss of generality.

In the following we assume  $J > 0$  ( $J$  acts as the energy scale). The properties of the model depend then on the value of  $\Delta$ .

#### \* FERROMAGNETIC PHASE ( $\Delta < -1$ )

- If  $\Delta < -1$  the XXZ chain is in the ferromagnetic Jahn phase: the ground state is the saturated state with all spins aligned along  $z$  or  $-z$ , i.e. the classical ground state with total magnetization  $S_{\text{tot}}^z = \pm N/2$  ( $N = \text{number of sites}$ ). This is thus a state with broken discrete symmetry, namely the specular symmetry  $S^z \leftrightarrow -S^z$ , under which  $\hat{H}$  is invariant.

Note: For  $\Delta = -1$  one recovers the full rotational symmetry of the isotropic Heisenberg model, recall p. 63).

The low-lying excited states in the ferromagnetic phase are magnons

- with  $S_{\text{tot}}^z = \frac{N}{2} - 1$  and dispersion law

$$E(q) = 2JS(1 - \cos q - (\Delta + 1))$$

Note: for  $\Delta = -1$  we recover the result of p. 63 in 1D

Note that at  $q=0$  there's a gap of magnitude  $|\Delta|-1$  for  $\Delta < -1$ .

At  $\Delta = -1$ , as we mentioned above, the discrete symmetry becomes continuous and the spectrum becomes gapless (recall our discussion on the Goldstone theorem in p. 64)

### • NÉEL PHASE ( $\Delta > 1$ )

- For  $\Delta \gg 1$  the XXZ chain is in the Néel phase (Ising AF). This phase presents in the thermodynamic limit broken symmetry and one finds 2 degenerate ground states (the  $S=1/2$  remnants of the classical Néel states,  $\dots \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \dots$ ). The ground states have  $S_{tot}^z = 0$ , but finite staggered magnetization:  $S_{stagg}^z = \sum (-1)^n S_n^z$  (and long-range order in the corresponding correlation function).

In contrast to the FM (as we already mentioned in p. 61) quantum fluctuations prevent a complete order (as one has in the classical Néel states).

For periodic boundary conditions and large but finite number of sites (which is the typical situation in the numerical analysis of these systems), the two ground states mix, leading to a ground state and an excited state separated by an energy  $gap \propto e^{-N}$ . The ground state has now translational invariance by the lattice site (and not by 2 lattice sites as the Néel states or the ground states for an infinite system).

The elementary excitations of this phase are easier to understand starting in the  $\Delta \rightarrow \infty$  limit (Ising limit). We may then start from one of the two ideal Néel states:

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

$\uparrow \downarrow \uparrow \boxed{\downarrow \downarrow} \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow$

$\uparrow \downarrow \uparrow \boxed{\downarrow \downarrow} \uparrow \downarrow \uparrow \boxed{\downarrow \downarrow} \uparrow \downarrow$

Let's turn around one spin. This breaks two bonds and lead to a state with energy  $\Delta$

Under repeated action of the Hamiltonian the state decays into two domain walls

These states are not any more eigenstates when  $\frac{1}{\Delta}$  is finite, but for  $\Delta \gg 1$  we can use perturbation theory. Up to  $\mathcal{O}(1/\Delta)$  one gets an excitation spectrum

$$\omega(q, \bar{\Phi}) = \Delta + 2 \cos q \cos 2\bar{\Phi} = \epsilon\left(\frac{q}{2} + \bar{\Phi}\right) + \epsilon\left(\frac{q}{2} - \bar{\Phi}\right)$$

(95)

$$\text{with } \epsilon(k) = \frac{\Delta}{2} + \cos 2k$$

where  $q$  is the total momentum [ $q = \frac{2\pi l}{N}$ ,  $l = 1, 2, \dots, N/2$ ]

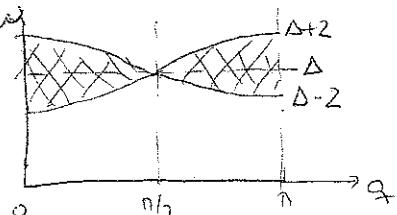
$\bar{\Phi}$  is the wave vector related to the superposition of domain walls with different distances [for  $S_{tot}^2 = \pm 1 \rightarrow \bar{\Phi} = \frac{M\pi}{N+2}$ ,  $M = 1, 2, \dots, N/2$ ]

[Note:  $\bar{\Phi}$  is essentially a relative momentum, but taking into account that the 2 domain walls can't penetrate each other]

The form of  $\omega(q, \bar{\Phi})$  shows that the excitation spectrum is composed by 2 entities, domain walls with dispersion  $\epsilon(k)$  and  $k_{1,2} = \frac{q}{2} \pm \bar{\Phi}$ . These domain walls constitute the so-called magnetic quantum solitons.

The elementary excitations in the Ising AF phase thus form a continuum with the relative momentum of the two domain walls as an internal degree of freedom.

### • XY PHASE ( $-1 < \Delta < 1$ )



For  $\Delta$  in this regime the system is in the XY phase. A full analysis of the XY phases may be achieved by means of Bethe Ansatz and bosonization. An approach in simpler terms may be obtained by means of the so-called Wigner-Jordan transformation, which maps  $S=1/2$  spin operators into spinless fermions ( $c_n$ ):

$$S_n^+ = c_n^+ e^{i\pi \sum_{p=1}^{n-1} c_p^+ c_p^-}$$

$$S_n^\pm = c_n^+ c_n^- - \frac{1}{2}$$

When a fermion is present/absent at a site  $n$ , the spin projection is  $S_n^z = +1/2 / -1/2$ .

[Note: naively we would have taken  $S^+ = c^+$ ,  $S^- = c$ , and  $S^z = c^+ c - 1/2$ . This transformation keeps the proper spin commutation rules (if  $c, c^\dagger$  are fermionic). But there's a problem. Spin operators at different sites must commute, which is not fulfilled by the naive mapping. The price to pay is that in the WJ-transformation every  $S_n^+$  has now attached a string of operators, and hence the mapping is clearly non-local].

The non-local character of the WO-transformation is however no problem

$$S_{n+1}^+ S_n^- = C_{n+1}^+ e^{i\pi \sum_{p=1}^n C_p^+ C_p^-} e^{-i\pi \sum_{p=1}^{n-1} C_p^+ C_p^-} C_n^+ = C_{n+1}^+ e^{i\pi C_n^+ C_n^-} C_n^+$$

But  $e^{i\pi C_n^+ C_n^-} C_n = \begin{cases} \text{if applied over } |N_n=0\rangle \rightarrow \text{it gives zero} \\ \text{if applied over } |N_n=1\rangle \rightarrow e^{i\pi C_n^+ C_n^-} |C_n=1\rangle = e^{i\pi C_n^+ C_n^-} |0\rangle = |0\rangle \end{cases}$

$$\text{Hence } e^{i\pi C_n^+ C_n^-} C_n = C_n$$

$$\text{Thus: } S_{n+1}^+ S_n^- = C_{n+1}^+ C_n^-$$

We may hence easily re-write the XXZ Hamiltonian in terms of the fermionic operators:

$$H_{XXZ} = J \sum_n \left\{ \frac{1}{2} (C_n^+ C_{n+1}^- + C_{n+1}^+ C_n^-) + \Delta (C_n^+ C_n^- - \frac{1}{2}) (C_{n+1}^+ C_{n+1}^- - \frac{1}{2}) \right\}$$

For general  $\Delta$  the XXZ chain is thus equivalent to an interacting 1D fermion system.

In the simplest case of  $\Delta=0$  (the XX model we have encountered for hard-core bosons in absence of dipolar interactions, recall p. 68) we have

$$H_{XX} = J \sum_n (C_n^+ C_{n+1}^- + C_{n+1}^+ C_n^-),$$

i.e. a non-interacting fermionic chain. For periodic boundary conditions we may introduce the Fourier transform ( $C_n = 1/\sqrt{N} \sum_k e^{ikn} c_k$ ) to get

$$H_{XX} = J \sum_k \cos k \, c_k^+ c_k^-$$

The assembly of free fermions is fully described by the dispersion law

$$\epsilon(k) = J \cos k$$

The ground state is then given by the free Fermi sea, i.e. all levels with  $\epsilon(k) \leq 0$  occupied. The Fermi wavevector is  $k_F = \pi/2$  and the total ground-state magnetization vanishes.

\* Low-lying excitations are simply described in the fermion picture.

We may:

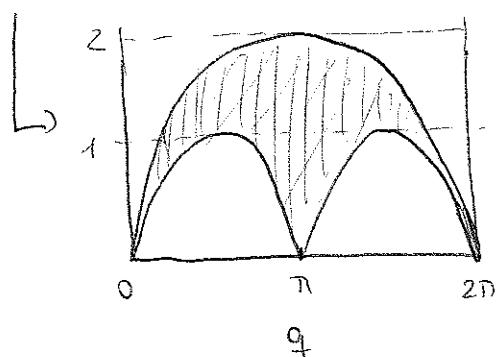
- (i) Add/remove fermions, thus changing the total magnetization  $S_{\text{tot}}^z$  by one unity and adding/removing  $\epsilon(\mathbf{k})$
- (ii) Create particle-hole excitations which do not change  $S_{\text{tot}}^z$ .

Creating a particle-hole excitation involves moving a fermion with  $\mathbf{k}_i$  inside the Fermi sea to some  $\mathbf{k}_f$  outside. It's clear that moving a fermion across the Fermi point (i.e. the "Fermi-surface" in 1D) cost arbitrarily low energy, and hence the spectrum is gapless.

For a given total momentum  $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$  there's a finite range of excitations energies possible:

$$\omega(\mathbf{q}, \mathbf{k}) = \epsilon(\mathbf{k} + \mathbf{q}) - \epsilon(\mathbf{k})$$

The spectrum of particle-hole excitations is hence a continuum with the initial momentum  $\mathbf{k}_i = \mathbf{k}$  as "internal" degree of freedom.



There are  $S_{\text{tot}}^z = 0$  excitations.  $S_{\text{tot}}^z = 1$  excitations have the same form but shifted by  $\pi$  along  $\mathbf{q}$ .

\* We will not discuss a general  $\Delta$ , but it's perhaps relevant to mention the isotropic Heisenberg AF ( $\Delta=1$ ). One may use Bethe-Ansatz techniques to find the ground state energy

$$E_0 = -N J \ln 2$$

Spin-spin correlation decay as  $\langle 0 | (-1)^n \vec{S}_n \cdot \vec{S}_0 | 0 \rangle \propto \frac{\sqrt{\ln n}}{n}$   
(i.e. dominantly as  $1/n$ )

As for the  $\Delta=0$  case the elementary excitations form a particle-hole continuum  $\omega(\mathbf{q}, \mathbf{k}) = \epsilon(\mathbf{q} + \mathbf{k}) - \epsilon(\mathbf{k})$  with

$$\epsilon(\mathbf{k}) = \frac{\pi}{2} J / \sin(k)$$

→ Spinon spectrum

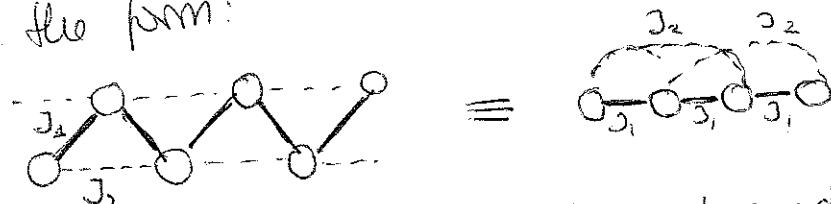
- At  $\Delta=1$  the system undergoes a phase transition from the gapless XY-phase to the gapped Ising AF. This transition is of the Kosterlitz-Thouless type, i.e. the excitation gap opens up with a nonanalytic dependence on  $\Delta-1$  corresponding to a correlation length:  $\xi \propto e^{\pi/\sqrt{\Delta-1}}$  (which determines the exponential decay of spin-spin correlations in the Ising AF)

### J1-J2 MODEL. MAJUNDAR-GHOSH LIMIT. DIMERIZATION

- Modifications of the XXZ chain may lead to an interesting physics. A theoretically particularly important model is the isotropic Heisenberg chain with nearest and next-nearest exchange:

$$\hat{H} = J \sum_n (S_n \cdot S_{n+1} + \alpha S_n \cdot S_{n+2}) \quad \xrightarrow{\text{This is the so-called } J_1-J_2 \text{ model}} \quad (J_1=J, J_2 \equiv J\alpha)$$

- Such models may be achieved in e.g. zig-zag optical lattices of the form:



These type of lattices may be achieved using techniques as those discussed in previous lectures. For example we may combine a triangular lattice (p.85) with an additional superlattice which splits the triangular lattice into separated zig-zags. Using the technique discussed in p.86 we may easily control  $J_1$  and  $J_2$ , and hence the value of  $\alpha$  in the previous Hamiltonian.

- If  $\alpha > 0$  the system exhibits frustration from competing interactions (recall p.87).
- The properties of the  $J_1-J_2$  model, and in particular the idea of spontaneous dimerization, are better understood by considering the special limit  $\alpha=1/2$  (Majundar-Ghosh limit):

$$\mu_{\text{MG}} = \sum_n (\vec{s}_n \cdot \vec{s}_{n+1} + \frac{1}{2} \vec{s}_n \cdot \vec{s}_{n+2}) \quad (\text{where we take } J=1)$$

let's consider the Hamiltonian

$$\begin{aligned}\tilde{H}_{\text{MG}} &= \frac{1}{4} (\vec{s}_1 + \vec{s}_2 + \vec{s}_3)^2 + \frac{1}{4} (\vec{s}_2 + \vec{s}_3 + \vec{s}_4)^2 + \frac{1}{4} (\vec{s}_3 + \vec{s}_4 + \vec{s}_5)^2 + \dots \\ &= \underbrace{\sum_n \vec{s}_n \cdot \vec{s}_{n+1} + \frac{1}{2} \sum_n \vec{s}_n \cdot \vec{s}_{n+2}}_{H_{\text{MG}}} + \frac{3}{4} \sum_n \vec{s}_n^2 \xrightarrow{\text{L}} \frac{3}{4}\end{aligned}$$

$$\text{Hence } H_{\text{MG}} = \tilde{H}_{\text{MG}} - \frac{9}{16} N$$

- \* let's consider each triplet  $\vec{s}_1 + \vec{s}_2 + \vec{s}_3 = \vec{s}_{123}$
- Recall that  $\vec{s}_{12} = \vec{s}_1 + \vec{s}_2$  may be a
  - singlet  $s_{12} = 0$
  - triplet  $s_{12} = \pm 1$
- Hence  $\vec{s}_{123}$  may be
  - $s_{123} = \frac{1}{2}$
  - $s_{123} = \frac{3}{2}$

$$\text{Hence } (\vec{s}_1 + \vec{s}_2 + \vec{s}_3)^2 \geq \frac{3}{4}$$

- \* Consequently the ground-state energy of  $\tilde{H}_{\text{MG}}$  must fulfill

$$E_0 \geq \frac{3}{16} N$$

- \* One may easily see that there are 2 degenerated ground states with energy  $\frac{3}{16} N$  obtained by averaging the chain completely with singlets:

$$|0\rangle_I = |[1,2], \dots, [2p+1, 2p+2], \dots \rangle \Rightarrow \text{Diagram of a chain with alternating singlets}$$

$$\text{and } |0\rangle_{II} = |[2,3], \dots, [2p, 2p+1], \dots \rangle \Rightarrow \text{Diagram of a chain with alternating singlets}$$

with the representation of the singlet

$$|[2p, 2p+1]\rangle = \frac{1}{\sqrt{2}} \sum_{ss'} x_{2p}(s) \epsilon^{s,s'} x_{2p+1}(s')$$

with  $x_m(s)$  the spin state at site  $m$

$\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$  the antisymmetric tensor.

- It's easy to see that for both states, each trio  $\vec{S}_n + \vec{S}_{n+1} + \vec{S}_{n+2}$  contains two spins which are coupled in a singlet and hence

$$(\vec{S}_n + \vec{S}_{n+1} + \vec{S}_{n+2})^2 = \frac{3}{4}$$

The other product states are therefore ground states of the Majumdar-Ghosh Hamiltonian with energy  $E_0 = -\frac{3}{8} N$ .

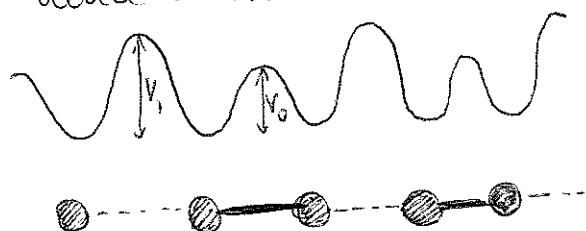
- The MG-Hamiltonian is hence characterized by a spontaneous dimerization. For a general  $\alpha$ , the  $J_1-J_2$  Hamiltonian presents spontaneous dimerization for  $\alpha > \alpha_c \approx 0.2411\dots$ . As for the MG case, this dimerized state is characterized by a singlet ground state with double lattice constant and twofold degeneracy, as well as an excitation gap to the first excited states (a band of triplets).

- Another variant of the Heisenberg chain is obtained by adding dimerization explicitly:

$$\hat{H} = J \sum_n (1 + (-1)^n \delta) (\vec{S}_n \cdot \vec{S}_{n+1}) \Rightarrow \text{---} \overset{\substack{\text{(weak bond)} \\ \delta(1-\delta)}}{\underset{\substack{\text{(strong bond)} \\ \delta(1+\delta)}}{\text{---}}} \text{---} \overset{\substack{\text{(weak bond)} \\ \delta(1-\delta)}}{\underset{\substack{\text{(strong bond)} \\ \delta(1+\delta)}}{\text{---}}} \text{---}$$

With explicit dimerization the ground state is unique, since the singlets are located at the strong bonds, and the excitation gap opens up immediately as  $E_g \propto \delta^{2/3}$ .

- Chains with explicit dimerization may be realized relatively easily using optical lattices, by combining 2 lattices with spacing  $a$  and  $2a$ . One hence obtains



By controlling the ratio  $\frac{V_1}{V_2}$  one may control as well the value of  $\delta$

[Note: We consider here of course a strong confinement in the other 2 directions, which may be attained by using a 2D square lattice. We consider as well the super-exchange scenario discussed in p 38.]

## \* SPIN CHAIN WITH S=1. HALDANE CHAIN.

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- \* Haldane discovered in the 80's that <sup>integer and half-integer-S</sup> antiferromagnetic Heisenberg spins behave in a very different way. He showed that the ground state of an integer-S Heisenberg AF chain should be gapped, presenting exponentially decaying AF spin correlations. This is the so-called Haldane phase, which we will briefly discuss for the S=1 case (Haldane chain) [i.e. isotropic S=1 Heisenberg AF]
- \* The Haldane chain is characterized (in its ground state) by short-range AF spin correlations

$$\langle S_0^x S_n^y \rangle \propto (-1)^n \delta_{xy} \frac{1}{\sqrt{n}} e^{-n/\xi} \quad \text{with } \xi \approx 6.$$

Its low-lying excitations fulfill the dispersion

$$E(q) = \sqrt{\Delta^2 + v^2(q-\pi)^2} \quad \text{with } \Delta \approx 0.41 J \rightarrow \text{gap} \\ v \approx 2.46 J \rightarrow \text{spin-wave velocity}$$

- \* An important property of the S=1 Haldane chain is the so-called string order which is a nonlocal quantity defined as the limiting value

$$O_{ST}^x = \lim_{|n-n'| \rightarrow \infty} \left\langle -S_n^x e^{i\pi \sum_{j=n+1}^{n'-1} S_j^x S_{j+1}^x} \right\rangle \quad \text{with } x=x,y,z$$

The presence of this order means that the ground state of the chain favors spin states where the  $\uparrow$  and  $\downarrow$  spin-1 states alternate "diluted" with strings of  $|0\rangle$  of arbitrary length. Something like this:  
 $\dots 0+0\dots 0-0\dots 0+0\dots 0-0\dots 0+0\dots \Rightarrow$  One speaks about a  
"diluted AF order"

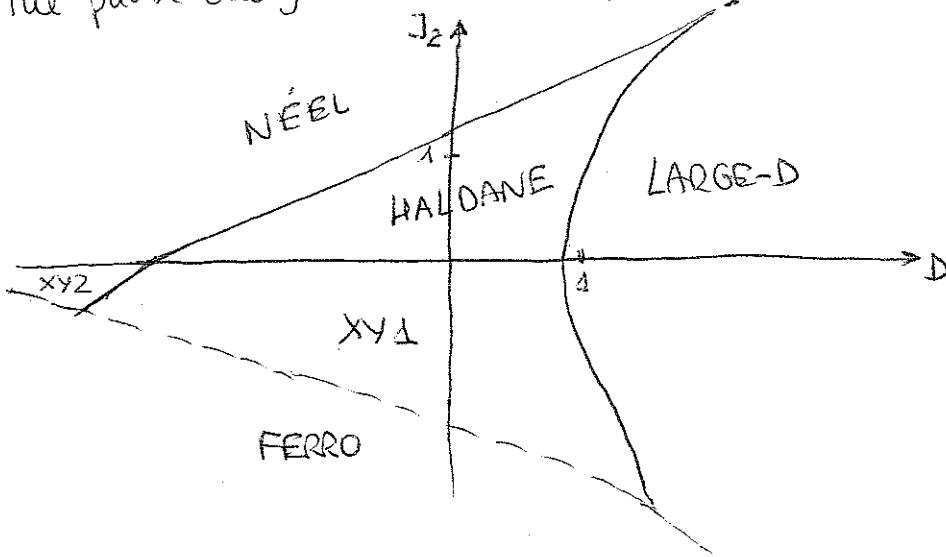
- \* This diluted AF order is maximal (and equal to 1) in the Néel state. In the Haldane phase, however, the Néel order vanishes, while the string order persists (the Néel order is killed by the lack of spatial ordering of the spins). For the Haldane chain  $O_x^{\text{HALD}} \approx 0.37$ .

\* An interesting phase diagram (of relevance e.g. for polar molecules, as we will see in a moment) emerges if one considers a  $S=1$  chain with anisotropies!

$$H = \sum_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + J^z S_n^z S_{n+1}^z + D(S_n^z)^2 \quad (\beta_{xy} = 1)$$

where we recognize the single-ion anisotropy ( $D(S_z^z)^2$ ) introduced in p. 89.

\* The phase diagram looks as follows:-



\* To visualize the characteristic features of the different phases it's useful to consider the  $| \pm \rangle$  spin states as occupied sites with spin  $\{ \uparrow, \downarrow \}$  and the  $| 0 \rangle$  sites as unoccupied sites.

Let's try then to visualize the different phases:

• Néel: in the visualizing picture is like an "AF spin-ordered solid"

$$+\downarrow -\uparrow +\downarrow -\uparrow +\downarrow -\uparrow \rightarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow$$

We have a phase with  
 1. long-range correlation of "particle positions"  
 2. long-range AF order of their "spins"

• Haldane phase: is like an "AF spin-ordered fluid"

$$\cdots +\downarrow 0 \cdots 0 -\downarrow 0 \cdots 0 +\downarrow 0 \cdots 0 -\downarrow \cdots \rightarrow \uparrow \times \times \downarrow \times \cdots \times \uparrow \times \cdots \times \downarrow$$

This phase has  
 1. no order in the "particle position"  
 2. AF order in "spin"

• XY1 phase: is like a "spin-disordered fluid" ↗ no order in "spin"

• XY2 phase: is like a "spin-disordered solid" ↗ order in "position" ↗ no order in "spin"

- Large-D phase: can be characterized as a gas of bound pairs of "particles" with opposite spin

$$|000\dots 00\rangle + |00\dots 0\oplus 0\dots 0\ominus 0\dots 0\rangle \dots$$

- Ferro phase: domains with either +, or -

\* These phases are quite generic for integer  $S$ . For half-integer  $S$  the large-D and Haldane phases disappear, being replaced by the XY1 phase.

### \* POLAR Bosons in 1D OPTICAL LATTICES: HALDANE-INSULATOR PHASE

- Interestingly a similar phase as the Haldane phase has been recently proposed in the context of polar bosons in optical lattices (recall p. ②) [E. Dalla Torre, E. Berg and E. Altman, PRL 97, 260401 (2006)].
- As in our discussion of p. ② we will just consider nearest-neighbor interactions:

$$\hat{\mu} = -t \sum_i (\hat{b}_i^\dagger \hat{b}_{i+1} + \hat{b}_{i+1}^\dagger \hat{b}_i) + \frac{U_0}{2} \sum_i \hat{n}_i (\hat{n}_{i-1}) + U_1 \sum_i \hat{n}_i \hat{n}_{i+1}$$

We consider in particular the case of unit filling, i.e.  $\bar{n}=1$  (equal number of particles and sites).

- This system resembles to a large extend a spin-1 chain, if we restrict to up to 2 particles per site:  $n_i = 0, 1, 2$ . We may then perform a Holstein-Primakoff transformation as in p. ②. We define:

$$\left. \begin{aligned} S_i^z &= 1 - \hat{n}_i \\ S_i^+ &= \sqrt{2 - \hat{n}_i} \hat{b}_i \\ S_i^- &= \hat{b}_i^\dagger \sqrt{2 - \hat{n}_i} \end{aligned} \right\} \rightarrow b_i^\dagger b_{i+1} = b_i^\dagger (2 - n_i)^{1/2} (2 - n_i)^{1/2} (2 - n_{i+1})^{1/2} (2 - n_{i+1})^{1/2} b_{i+1}$$

$$= S_i^+ (1 + S_i^z)^{-1/2} (1 + S_i^z)^{-1/2} S_{i+1}^+$$

The Hamiltonian may be then re-written in the form:

$$\hat{H} = -E \sum_i \left[ S_i^+ (S_i^z + 1)^{1/2} (S_{i+1}^z + 1)^{-1/2} S_{i+1}^+ + \text{U.C.} \right] + \frac{U_0}{2} \sum_i (1 - S_i^z)(1 - S_{i+1}^z)$$

$$+ U_1 \sum_i (1 - S_i^z)(1 - S_{i+1}^z)$$

(104)

\* Eliminating constants (since  $\sum_i S_i^z = \text{constant}$ ) we retrieve:

$$\hat{H}_{\text{eff}} = -2t \sum_i \frac{1}{2} (S_i^- S_{i+1}^+ + S_{i+1}^- S_i^+) + U_1 \sum_i S_i^z S_{i+1}^z + \frac{U_0}{2} \sum_i (S_i^z)^2 \\ - t \sum_i [S_i^- F(S_i^z + S_{i+1}^z) S_{i+1}^+ + \text{h.c.}]$$

$$\text{where } F(S^z) = \left(\frac{1-\sqrt{2}}{\sqrt{2}}\right) \delta_{S^z,1} + \left(\frac{-1}{2}\right) \delta_{S^z,2}$$

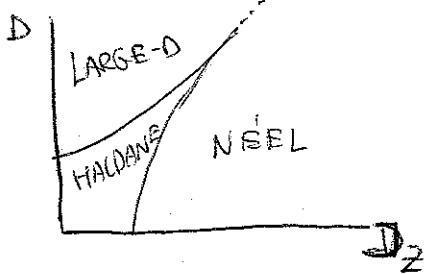
\* Neglecting the term of the 2<sup>nd</sup> line one gets a spin-1 Hamiltonian.  
Introducing the usual transformation  $S_{i \in B}^{x,y} \rightarrow -S_{i \in B}^{x,y}$  for the B sublattice

We get

$$H_{\text{eff}}^{S=1} = 2t \sum_i [(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \frac{U_1}{2t} S_i^z S_{i+1}^z + \frac{U_0}{4t} (S_i^z)^2]$$

We recognize the same Hamiltonian as in p. (102) with  $J=2t$  and  
 $J_z = U_1/2t$  and  $D = U_0/4t$ .

\* Recall that for  $J_z > 0$  and  $D > 0$  (as it's the case now)  
the  $S=1$  chain presents the phase diagram:



\* The equivalent of the large- $D$  phase ( $|S_i^z=0\rangle \Rightarrow 10,0,\dots 0\dots$ )  
is in the bosonic language the Mott-insulator phase (MI)



\* The equivalent of the Néel phase is a "charge density wave" (CDW)



\* One may then expect the existence of a Haldane-Mott phase, which  
has been called the Haldane-insulator phase (HI)

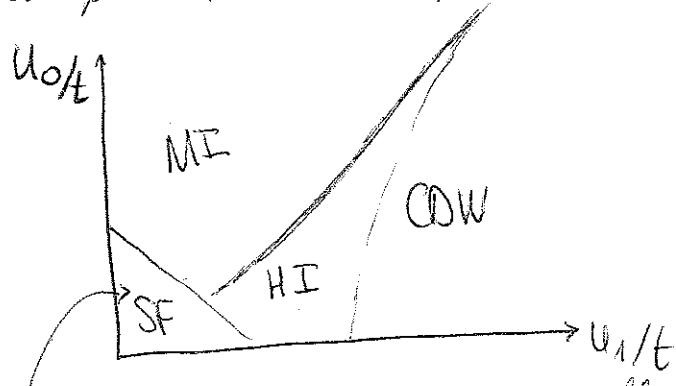
\* the Haldane-Mottluer phase is characterized by nesting order: (105)

$$\Omega_{SI} = \lim_{|i-j| \rightarrow \infty} \left\langle \delta n_i (-1)^{\sum_{l=i+1}^{j-1} \delta n_l} \delta n_j \right\rangle \quad \text{with } \delta n_i = 1 - n_i$$

This phase may be sketched as:

2 1 ... 1 0 1 ... 1 2 1 ... 1 0  
<sup>1</sup>  
# of particle interact site

\* This phase has been found indeed in DMRG calculations



a superfluid regime appears as well at low  $\frac{V_0}{t}, \frac{V_1}{t}$  as one would expect.

[Note: The HI phase survives even if we consider interactions beyond nearest neighbor, and occupations  $> 2$ ].

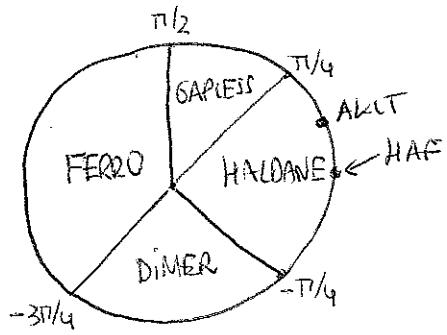
### \* $S=1$ BILINEAR-BIQUADRATIC CHAIN

\* As we saw in p. (10), the isotropic Heisenberg  $S=1$  AF chain is a generic example of a system in the Haldane phase. However, the most general isotropic exchange interaction for  $S=1$  includes biquadratic terms as well, being of the form

$$H = \sum \cos \Theta (\vec{S}_n \cdot \vec{S}_{n+1}) + g \mu \Theta (\vec{S}_n \cdot \vec{S}_{n+1})^2 \xrightarrow{\substack{\text{Bilinear-Biquadratic} \\ \rightarrow S=1 \text{ Hamiltonian}}}$$

\* Recall that this Hamiltonian may be achieved in  $S=1$  spinor lattice gases (p. 84) [Note: Unfortunately the spinor gas just allows for studying  $\Theta$  in a regime  $\Theta_0 < \Theta < 30^\circ$ , where  $\Theta_0$  is slightly larger than  $\pi$ . There are some ideas, however, based on the idea of inverted Hamiltonian (and TCO) which may allow other  $\Theta$ 's]

\* The ground-state properties of this Hamiltonian depend crucially on the value of the angle  $\Theta$ :



- \*  $-\pi/4 < \theta < \pi/4 \rightarrow \underline{\text{Haldane phase}}$   
(i.e. gapped and with strong order)
- \*  $\pi/2 < \theta < \frac{3\pi}{4} \rightarrow \underline{\text{Ferromagnetic phase}}$
- \*  $\pi/4 < \theta < \pi/2 \rightarrow \underline{\text{gapless phase}}$   
(at  $\pi/4$  there's a BKT transition from the gapped Haldane to the gapless phase)
- \*  $-3\pi/4 < \theta < \pi/4 \rightarrow \underline{\text{Dimer phase}}$   
Spontaneously dimerized phase (recall p. 42), gapped.

\* For  $\tan \theta = 1/3$  one obtains the so-called AKLT model:

$$H_{\text{AKLT}} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \sum_i (\vec{S}_i \cdot \vec{S}_{i+1})^2$$

This model is particularly interesting, being the prototype of the so-called valence bond solid (VBS) models. It's especially useful to understand some interesting ideas concerning the Haldane phase.

\* Let's introduce the projectors  $P_{12}^{(J)}$  which project the states of two spins  $\vec{S}_1$  and  $\vec{S}_2$  onto the subspace with total spin  $J$ .

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2} [J(J+1) - 4] \begin{cases} -2 & (S=0) \\ -1 & (S=1) \\ 1 & (S=2) \end{cases}$$

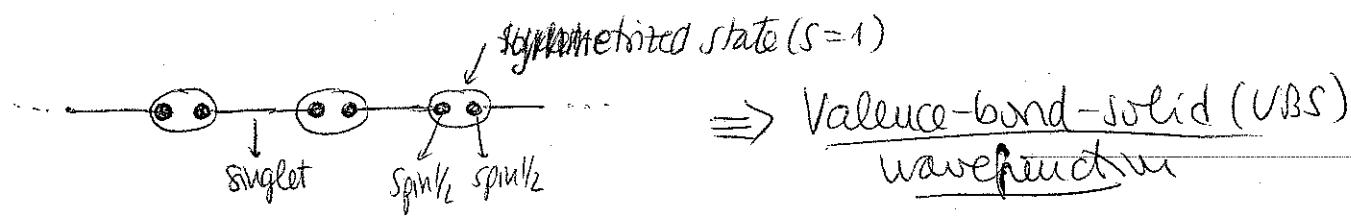
$$\text{Then: } (\vec{S}_1 \cdot \vec{S}_2) + \frac{1}{3} (\vec{S}_1 \cdot \vec{S}_2)^2 = -\frac{2}{3} (P_{12}^{(0)} + P_{12}^{(1)}) + \frac{4}{3} P_{12}^{(2)} = 2 P_{12}^{(2)} - \frac{2}{3}$$

Hence

$$H_{\text{AKLT}} = \sum_i \left\{ 2 P_{i,i+1}^{(2)} - \frac{2}{3} \right\}$$

It becomes very clear that the minimum energy is obtained for a state such that the total spin of any two neighboring spins is never equal to 2.

\* Such a state can be constructed by regarding every  $S=1$  spin or a composite of two symmetrized  $S=1/2$  spins, and coupling each  $S=1/2$  spin to its neighbor from the nearest site with a singlet bond



• For periodic boundary conditions the ground state is unique, being a global singlet.

For open boundary conditions there are two free spin- $\frac{1}{2}$  spins at the open ends. The ground-state is hence fourfold degenerate, since the free edge spins may form a singlet and a triplet. These are the so-called edge states.

• Interestingly, there exists a simple and elegant representation of VBS wavefunctions using the language of matrix product states (MPS):

$$|\Psi\rangle_{\text{AKLT}} = \text{Tr}(g_1 g_2 \dots g_N) \quad \text{with} \quad g_n = \frac{1}{\sqrt{3}} \begin{bmatrix} -10\rangle_n & -\sqrt{2}1-\rangle_n \\ \sqrt{2}1+\rangle_n & 10\rangle_n \end{bmatrix}$$

The trace corresponds to periodic boundary conditions, and the four matrix elements of  $\Sigma = g_1 \dots g_N$  are the four degenerate ground states of the open chain

• The MPS representation makes it easy to see the appearance of string order in the VBS wave function. We may re-write

$$g_n = \frac{1}{\sqrt{3}} [\sigma^+ |-\rangle_i + \sigma^- |+\rangle_i - \sigma^z |0\rangle_i] \quad \text{with } \sigma^\pm, \sigma^z \text{ the Pauli matrices.}$$

• Since  $(\sigma^\pm)^2 = 0$  and  $\sigma^\pm \sigma^\pm = \mp \sigma^\pm$ , the ground-state  $|\Psi\rangle_{\text{AKLT}}$  contains only states where a  $|+\rangle$  must be followed by a  $|-\rangle$ , with an arbitrary number of  $|0\rangle$  in between. The "diluted AF order" of p. 101 is hence perfect in the AKLT model, with  $\Omega_1^{\text{AKLT}} = 4/9$

• Note: The AKLT state is rotationally invariant, and hence  $|0\rangle, |+\rangle, |-\rangle$  have equal probability  $1/3$ . A non-zero contribution to  $\Omega_1$  occurs only when  $S_{n,n'} = \pm 1$ , which occurs with probability  $4/9$ . Hence  $\Omega_1^{\text{AKLT}} = 4/9$  is the maximal value of  $\Omega_1$  for a rotational invariant state. Recall that  $\Omega_1^{\text{Haldane}} = 0.37$ . [p. 101]

• The hidden order (i.e. the non-local string order), together with the four-fold degeneracy of the ground state for open chains, are characteristic features of the Haldane phase for  $S=1$  chains.

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• Of course there are much more significant models in 1D, and much more scenarios than those discussed here. The goal here was just to show few prototypical examples which (to a large extent) may be realized with ultra-cold gases in optical lattices, using the techniques discussed in previous lectures.

One should mention, of course, that there are other highly interesting scenarios in higher-dimensional geometries, which we will not discuss here.

• Atoms in optical lattices offer hence a very exciting system for the controlled analysis of strongly-correlated systems!