Haldane-gap chains in a magnetic field

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Abstract. We consider quasi-one-dimensional spin-1 Heisenberg chains with crystal field anisotropy in a uniform magnetic field. We determine the dynamical structure factor in various limits and obtain a fairly complete qualitative picture of how it changes with the applied field. In particular, we discuss how the width of the higher energy single magnon modes depends on the field. We consider the effects of a weak interchain coupling. We discuss the relevance of our results for recent neutron scattering experiments on the quasi-1D Haldane-gap compound NDMAP.

Keywords: spin chains, ladders and planes (theory), correlation functions (theory), quantum phase transitions (theory)

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# Contents

1. Introduction .................................................. 3

2. Majorana fermion model ...................................... 4
   2.1. Symmetries ................................................... 5
   2.2. Spectrum in the absence of interactions .................... 5
   2.3. Interactions: self-consistent mean-field treatment .......... 8
   2.4. Decay processes in the low-field phase ..................... 8

3. Landau–Ginzburg (LG) model .................................. 10
   3.1. Spectrum and mode expansion ................................. 11
   3.2. Decay processes ............................................. 12

4. Vicinity of the Ising critical point .......................... 14
   4.1. $H < H_c$: low-field phase ................................... 16
   4.2. $H = H_c$: at criticality ..................................... 16
   4.3. $H > H_c$: high-field phase .................................. 17

5. The high-field phase for weak anisotropy .................... 17
   5.1. Spectrum of the SGM ........................................... 19
   5.2. Dynamical structure factor ................................. 20
      5.2.1. Spectral weights ........................................ 21
      5.2.2. Polarizations in the LG model .......................... 23

6. Interchain coupling .............................................. 24
   6.1. Mean-field approximation ................................... 25
      6.1.1. The limit $h \to 0$: McCoy–Wu scenario ................ 26
      6.1.2. The limit $m_0 \to 0$: magnetic deformation .......... 27
      6.1.3. Qualitative behaviour in the general case .......... 27
   6.2. Beyond mean-field: RPA ..................................... 28

7. Summary and discussion ....................................... 29

Acknowledgments .................................................. 30

Appendix A: Low-field phase in the absence of crystal field anisotropy 30
Appendix B: Spectral representation of correlation functions ........ 31
Appendix C: Bound states in the Majorana model .................. 32
Appendix D: Low-energy projections of the staggered magnetizations 33
   Appendix D.1. Landau–Ginzburg model ......................... 33
   Appendix D.2. Majorana fermion model ......................... 34
Appendix E: Derivation of the sine-Gordon model in the high-field phase for weak anisotropy 36
   Appendix E.1. Nonlinear sigma model ........................... 36
   Appendix E.2. Majorana fermion model ......................... 37
1. Introduction

Recent years have seen a resurgence of interest in field-induced ‘magnon condensation’ in gapped quasi-one-dimensional quantum antiferromagnets. In particular a series of ESR and neutron scattering experiments have been carried out on the Haldane-gap [1] chain compounds NDMAP [2]–[7] and NDMAZ [8]. The main motivation for these experimental studies is the observation that a spin-1 Heisenberg chain undergoes a quantum phase transition between a gapped spin-liquid phase and a gapless Luttinger liquid phase at some critical value \( H_c \) of the applied magnetic field \( H \) [9,10]. The ground state of the spin-1 Heisenberg chain is a spin singlet and excitations are described in terms of a gapped \( S = 1 \) triplet of magnons. When a magnetic field is applied, the triplet splits due to the Zeeman effect and one of the magnon gaps is driven to zero at \( H_c \). For \( H > H_c \) the ground state is magnetized and excitations are gapless. If interactions between the magnons were absent, the transition at \( H_c \) could be understood as a Bose–Einstein condensation of magnons. In the spin-1 Heisenberg chain there is an interaction between magnons, which fundamentally changes the ground state for \( H > H_c \) from a condensate of bosonic magnons to a Luttinger liquid, which can be regarded as a one-dimensional version of an interacting Bose condensate. The transition at \( H = H_c \) is in the universality class of the commensurate–incommensurate (C–IC) phase transition [11]. The magnetic response of the isotropic spin-1 chain in strong fields \( H > H_c \) has been analysed in some detail in [12]–[14]. In appendix A we use the nonlinear sigma model description of the isotropic spin-1 chain to derive explicit expressions for the dynamical response functions in the low-field phase \( H < H_c \). In many \( S = 1 \) compounds such as NENP, NDMAP and NDMAZ strong crystal field anisotropies are present, which lead to a zero-field splitting of the magnon triplet comparable in magnitude to the Haldane gap itself. These anisotropy effects lead to more complex behaviour and a richer phase diagram. The purpose of this work is to determine the dynamical response of Haldane-gap compounds in the presence of such crystal field anisotropies. The relevant lattice Hamiltonian is of the form

\[
\mathcal{H} = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} - \mathbf{H} \cdot \mathbf{S}_j + \sum_j D(S^z_j)^2 + E[(S^x_j)^2 - (S^y_j)^2],
\]

where \( 0 < -E < D \). In zero field there are three magnon modes in the vicinity of the antiferromagnetic wavenumber \( q = \pi/a_0 \) with gaps \( \Delta_1 < \Delta_2 < \Delta_3 \). For simplicity we will mainly concentrate on the case where the magnetic field is applied along the \( z \)-axis, i.e.

\[
\mathbf{H} = H\hat{e}_z.
\]

The lattice Hamiltonian (1.1) (with field applied along the \( z \)-direction) exhibits two discrete symmetries which play an important role in the following:

1. Rotation by \( \pi \) around the \( z \)-axis (\( R^z_\pi \)):

\[
S^x_j \rightarrow -S^x_j, \quad S^y_j \rightarrow -S^y_j, \quad S^z_j \rightarrow S^z_j.
\]

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Haldane-gap chains in a magnetic field

(2) Translation by one site \((T_R)\):

\[
S^\alpha_j \rightarrow S^\alpha_{j+1}, \quad \alpha = x, y, z.
\]

The model (1.1) is difficult to analyse directly by analytical methods. However, progress can be made by concentrating on the low-energy regime, which can be studied by means of semi-phenomenological descriptions in terms of continuum models. Two such models have been used in particular, namely (i) a bosonic Landau–Ginzburg model [10, 14] and (ii) a theory of three coupled Majorana fermions [15]. In the present work we go beyond the original works [10, 14, 15] by (1) discussing the decay of high energy magnon modes, (2) applying methods of integrable quantum field theory to the discussion of structure functions and (3) taking into account the effects of interchain interactions.

The outline of this paper is as follows. We start by reviewing known results on the spectrum of the Majorana fermion model in section 2.2. We then investigate the role played by interactions in sections 2.3 and 2.4 and in particular show that interactions generate a finite lifetime for one of the magnon modes. In section 3 we derive analogous results in the framework of the Landau–Ginzburg theory. We then turn to a more detailed analysis of the magnetic response functions in the low-energy regime in the vicinity of the quantum critical point at \(H_c\) in section 4. Section 5 gives a detailed account of the low-energy regime in the high-field phase for small crystal-field anisotropy. The effects of interchain coupling are investigated in section 6 and a summary and discussion of our various results is given in section 7. A variety of technical details are presented in appendices A–E.

2. Majorana fermion model

In [15] Tsvelik proposed a description of the spin-1 Heisenberg chain in terms of a field theory of three right and left moving Majorana (real) fermions \(R_a = R^\dagger_a,\ L_a = L^\dagger_a,\ a = 1, 2, 3\). The Hamiltonian is given by

\[
\mathcal{H} = \frac{i}{2} \sum_{a=1}^{3} v [L_a \partial_x L_a - R_a \partial_x R_a] - \Delta_a [R_a L_a - L_a R_a] + \frac{i}{2} \sum_{a,b,c} \epsilon^{abc} H_a (L_b L_c + R_b R_c) + \mathcal{H}',
\]

where \(\mathcal{H}'\) describes anisotropic current–current interactions

\[
\mathcal{H}' = \sum_a g_a J^a J^a.
\]

Here the currents are bilinears in the Majorana fermions

\[
J^a(x) = -\frac{i}{2} \epsilon^{abc} [L_b L_c + R_b R_c].
\]

We will take the magnetic field along the three-axis and concentrate on the case

\[
\Delta_1 < \Delta_2 < \Delta_3.
\]
The generalization of our results to other situations is straightforward. The smooth and staggered components of the spin operators are defined by the decomposition

\[ S^\alpha_j \rightarrow J^\alpha(x) + (-1)^j n^\alpha(x), \]  

where \( x = ja_0 \). The smooth components are equal to the currents, where \( a = 1, 2, 3 \) corresponds to \( \alpha = x, y, z \). The staggered components are expressed in terms of Ising order and disorder operators

\[ n^x(x) \propto \sigma^1(x) \mu^2(x) \mu^3(x), \]
\[ n^y(x) \propto \mu^1(x) \sigma^2(x) \mu^3(x), \]
\[ n^z(x) \propto \mu^1(x) \mu^2(x) \sigma^3(x). \]

We note that the signs of the mass terms in (2.1) are such that in zero field

\[ \langle \sigma^a(x) \rangle = 0, \quad \langle \mu^a(x) \rangle \neq 0. \]  

2.1. Symmetries

The Hamiltonian (2.1) inherits the discrete symmetries \( T_R \) and \( R_z \pi \) from the lattice model. The latter is realized as

\[ R^a \rightarrow -R^a, \quad L^a \rightarrow -L^a, \quad \sigma^a \rightarrow -\sigma^a, \quad \mu^a \rightarrow \mu^a, \quad a = 1, 2. \]  

The translation symmetry by one site turns into a discrete \( Z_2 \) symmetry in the continuum limit

\[ J^a(x) \rightarrow J^a(x), \quad n^a(x) \rightarrow -n^a(x), \]  

and may be realized as

\[ R^a \rightarrow -R^a, \quad L^a \rightarrow -L^a, \quad \sigma^a \rightarrow -\sigma^a, \quad \mu^a \rightarrow \mu^a, \quad a = 1, 2, 3. \]  

It is convenient to combine this symmetry with \( R^z \) into the following \( Z_2 \) symmetry

\[ T_R R^z: \quad R^a \rightarrow -R^a, \quad L^a \rightarrow -L^a, \quad \sigma^3 \rightarrow -\sigma^3, \quad \mu^3 \rightarrow \mu^3. \]  

The full symmetry of the Majorana model (2.1) is thus \( Z_2 \otimes Z_2 \).

2.2. Spectrum in the absence of interactions

In the absence of interactions, i.e. \( g_a = 0 \) in (2.2) the Hamiltonian can be diagonalized by means of a Bogoliubov transformation \[15\]. In the following we review some relevant formulae. As the magnetic field is along the three direction only the first and second Majoranas couple to the magnetic field. The third Majorana gives rise to a fermionic single-particle mode with dispersion

\[ \omega_3(k) = \sqrt{\Delta_3^2 + v^2 k^2}. \]
The first and second Majoranas are conveniently combined into a complex fermion $\Psi$

$$R_1 = \frac{\Psi_R + \Psi_R^\dagger}{\sqrt{2}}, \quad R_2 = \frac{\Psi_R - \Psi_R^\dagger}{i\sqrt{2}},$$
$$L_1 = \frac{\Psi_L + \Psi_L^\dagger}{\sqrt{2}}, \quad L_2 = \frac{\Psi_L - \Psi_L^\dagger}{i\sqrt{2}}.$$  \hspace{1cm} (2.13)

The Hamiltonian density describing the first and second Majoranas takes the form

$$\mathcal{H}_{12} = -i v \left[ \Psi_R^\dagger \partial_x \Psi_R - \Psi_L^\dagger \partial_x \Psi_L \right] + \frac{H}{2} \left[ \Psi_R^\dagger \Psi_R + \Psi_L^\dagger \Psi_L \right]$$
$$- i m \left[ \Psi_R^\dagger \Psi_L - \text{h.c.} \right] + i \Delta \left[ \Psi_R^\dagger \Psi_L - \text{h.c.} \right],$$  \hspace{1cm} (2.14)

where

$$\Delta = \frac{\Delta_2 - \Delta_1}{2}, \quad m = \frac{\Delta_2 + \Delta_1}{2}. \hspace{1cm} (2.15)$$

Introducing a mode expansion

$$\Psi_R(x) = \int_0^\infty \frac{dk}{2\pi} \left[ e^{ikx} \alpha(k) + e^{-ikx} \beta^\dagger(k) \right],$$
$$\Psi_L(x) = \int_0^\infty \frac{dk}{2\pi} \left[ e^{ikx} \alpha(k) + e^{-ikx} \beta^\dagger(k) \right],$$  \hspace{1cm} (2.16)

we may express the Hamiltonian density (2.14) as

$$H_{12} = \int_0^\infty \frac{dk}{2\pi} \sum_{a,b=1}^4 \gamma_a^\dagger(k) M_{ab} \gamma_b(k),$$  \hspace{1cm} (2.17)

where

$$\gamma_a(k) = (\alpha(k),\alpha^\dagger(-k),\beta(k),\beta^\dagger(-k))_a,$$
$$M = \begin{bmatrix}
v k + H & i\Delta & 0 & -im \\
-i\Delta & -vk - H & \text{im} & 0 \\
0 & \text{im} & vk - H & i\Delta \\
im & 0 & -i\Delta & -vk + H
\end{bmatrix}. \hspace{1cm} (2.18)$$

Now we perform a Bogoliubov transformation with a unitary matrix $U(k)$

$$\begin{pmatrix} c_+(k) \\
 c_+^\dagger(-k) \\
 c_-(k) \\
 c_-^\dagger(-k) \end{pmatrix} = U(k) \begin{pmatrix} \alpha(k) \\
 \alpha^\dagger(-k) \\
 \beta(k) \\
 \beta^\dagger(-k) \end{pmatrix},$$  \hspace{1cm} (2.19)

to bring $H_{12}$ to a diagonal (normal ordered) form

$$H_{12} = \int_{-\infty}^\infty \frac{dk}{2\pi} \sum_{a=\pm} \omega_a(k) c_a^\dagger(k) c_a(k),$$
$$\omega_\pm(k) = \left[ m^2 + \Delta^2 + H^2 + v^2 k^2 \pm 2\sqrt{m^2 \Delta^2 + H^2 (m^2 + v^2 k^2)} \right]^{1/2}. \hspace{1cm} (2.20)$$
The gap $\omega_+(0)$ increases monotonically with $H$, whereas $\omega_-(0)$ decreases and vanishes at a critical field

$$H_c = \sqrt{\Delta_1\Delta_2} = \sqrt{m^2 - \Delta^2}. \quad (2.21)$$

The corresponding critical point is in the Ising universality class. For fields $H < H_{c2}$

$$H_{c2} = m \left[ \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{\Delta^2}{m^2}} \right]^{1/2} \quad (2.22)$$

the minimum of the dispersion $\omega_-(k)$ occurs at $k = 0$. In the vicinity of $H_c$ and at small momenta the dispersion is approximated as

$$\omega^2(k) \approx \frac{H_c^2}{m^2} (H - H_c)^2 + v^2 \left[ \frac{\Delta^2}{m^2} + \frac{H_c(1 + (\Delta^2/m^2))}{m^2}(H_c - H) \right] k^2. \quad (2.23)$$

Hence the gap vanishes linearly with $H - H_c$ in agreement with Ising critical behaviour

$$\omega_-(0) \approx (H - H_c) \sqrt{1 - \frac{\Delta^2}{m^2}}. \quad (2.24)$$

In order to see the Ising criticality described by (2.23) the magnetic field must be sufficiently close to $H_c$

$$H - H_c < \frac{\Delta^2}{H_c(1 + (\Delta^2/m^2))}. \quad (2.25)$$

As expected this scale is set by the anisotropy $\Delta$. For $H > H_{c2}$ there are two degenerate minima of $\omega_-(k)$ at some incommensurate wavenumbers $\pm k_F$ with

$$vk_F = \left[ H^2 - m^2 - \frac{m^2\Delta^2}{H^2} \right]^{1/2}, \quad (2.26)$$

$$\omega_-(k_F) = \Delta \sqrt{1 - \frac{m^2}{H^2}}.$$

For $k \approx \pm k_F$ we have

$$\omega^2(k) \approx \Delta^2 \left[ 1 - \frac{m^2}{H^2} \right] + \left[ \frac{v^2k_F}{H} \right]^2 (|k| - k_F)^2. \quad (2.27)$$

As was recently pointed out by Wang [26], these results for the dispersions suggest that a cross-over between Ising and C–IC critical behaviour occurs as a function of $H$. For $H$ very close to $H_c$ we encounter Ising critical behaviour, which crosses over to C–IC behaviour for $H > H_{c2}$. 

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[Image: J STAT (2004) P12006]
2.3. Interactions: self-consistent mean-field treatment

So far we have neglected the four-fermion interactions (2.2) altogether. As a first step of taking interactions into account we may treat them in a self-consistent mean-field (SCMF) approximation. The following expectation values are compatible with the discrete $Z_2$ symmetries

\[ \langle L_a R_a \rangle \neq 0, \quad \langle L_1 L_2 \rangle \neq 0, \quad \langle R_1 R_2 \rangle \neq 0, \quad \langle R_1 L_2 \rangle \neq 0, \quad \langle R_2 L_1 \rangle \neq 0. \]  

(2.28)

Decoupling the four fermion terms leads to a renormalization of the mass parameters

\[ \Delta_1 \rightarrow \tilde{\Delta}_1 = \Delta_1 - 2ig_2 \langle L_3 R_3 \rangle - 2ig_3 \langle L_2 R_2 \rangle, \]
\[ \Delta_2 \rightarrow \tilde{\Delta}_2 = \Delta_2 - 2ig_1 \langle L_3 R_3 \rangle - 2ig_3 \langle L_1 R_1 \rangle, \]
\[ \Delta_3 \rightarrow \tilde{\Delta}_3 = \Delta_3 - 2ig_3 \langle L_2 R_2 \rangle - 2ig_2 \langle L_1 R_1 \rangle. \]  

(2.29)

The magnetic field terms are changed to

\[ H_L L_1 L_2 + H_R R_1 R_2, \]  

(2.30)

where $H_L = H + 2ig_3 \langle R_1 R_2 \rangle$ and $H_R = H + 2ig_3 \langle L_1 L_2 \rangle$. Finally, two new terms are generated

\[ i\lambda_1 R_1 L_2 + i\lambda_2 L_1 R_2, \]  

(2.31)

where $i\lambda_1 = 2g_3 \langle L_1 R_2 \rangle$ and $i\lambda_2 = 2g_3 \langle R_1 L_2 \rangle$. The resulting mean-field Hamiltonian is quadratic in the Fermi fields and can again be diagonalized by a Bogoliubov transformation. Let us denote the ground state energy obtained in this way by $E_{GS}$. The expectation values are determined self-consistently, e.g.

\[ -i\langle R_a L_a \rangle = \frac{\partial E_{GS}}{\partial \tilde{\Delta}_a}. \]  

(2.32)

The SCMF procedure is easily implemented once the appropriate couplings $g_a$ are specified. However, in order to keep matters as simple as possible we will assume from now on that the $g_a$ are small and as a result the differences between the free theory and the SCMF theory are negligible. The main qualitative effect of nonzero $g_a$ is to make the gap of the third Majorana magnetic field dependent. Such a dependence is observed for example in experiments on NDMAP [4,5] and implies the presence of interactions in the framework of the Majorana fermion model.

2.4. Decay processes in the low-field phase

Within the SCMF approximation the role of the current–current interactions is merely to induce slight changes of the dispersion relations of the three coherent single-particle magnon modes. As we will now show, treating the interactions beyond the SCMF approximation leads to the damping of one of the magnons.

The analysis of the spectrum summarized above establishes that there are three different types of magnon, which we will refer to as $M_3$, $M_+$ and $M_-$, respectively. The corresponding dispersion relations are $\omega_3(k)$ (2.12) and $\omega_{\pm}(k)$ (2.20). The interaction of these modes is described by the term $H'$ in the Hamiltonian (2.1) and involves four particles. As $\omega_-(k)$ can become very small as the magnetic field is increased from zero,
the decays $M_3 \rightarrow M_-M_-M_-$ and $M_+ \rightarrow M_-M_-M_-$ become kinematically allowed for sufficiently large magnetic fields. However, the decay of $M_3$ is forbidden by the symmetry $T_R R^z$: $M_3$ is odd under this symmetry whereas $M_\pm$ are even. Essentially we are using the fact that all three magnon modes only exist near wavevector $\pi/a_0$ so that they can only decay into an odd number of magnons. The decay of $M_3$ into any odd number of $M_-$ is forbidden by the $R^z$ spin rotation symmetry. On the other hand the decay $M_+ \rightarrow M_-M_-M_-$ is allowed by symmetry. The process becomes kinematically possible as soon as the magnetic field exceeds a critical value $H_d$, which is defined by

$$\omega_+(0) = 3\omega_-(0).$$

Solving for $H_d$ we find

$$H_d = \sqrt{\frac{m^2}{4} - \Delta^2}.$$  \hspace{1cm} (2.34)

As long as $2\Delta < m$ the decay process will occur for $H > H_d$ and from now on we will assume that this is the case.

We note that in zero field there are no decay processes even if the gaps are such that they are kinematically allowed ($3\Delta_1 < \Delta_2$). The reason is that for $H = 0$ the lattice Hamiltonian (1.1) has additional spin rotational symmetries around the $x$ and $y$ axes by 180°. In combination with the translation symmetry these induce symmetries of the form (2.11) for the Majoranas 1 and 2 individually rather than the combination (2.8). This additional symmetry forbids decay processes.

Inserting the mode expansions (2.16) into the expression for $\mathcal{H}'$, integrating over the spatial coordinate and then carrying out the Bogoliubov transformation (2.19) generates several terms quartic in the fermionic creation annihilation operators $c_{\pm}(k)$, $c_{\pm}^\dagger(k)$. The most interesting one describes the decay of a $M_+$ mode into three $M_-$ modes and is of the form

$$V = g_3 \int_{-\infty}^{\infty} \frac{dk_1}{(2\pi)^3} f(k_1, k_2, k_3) c_-(k_1) c_-(k_2) c_-(k_3).$$

Here $f$ is an antisymmetric function of its arguments and at small momenta is of the form

$$f(k_1, k_2, k_3) \approx \tilde{C}(k_1 - k_2)(k_1 - k_3)(k_2 - k_3).$$

The constant $\tilde{C}$ is a complicated function of $\Delta$, $m$ and $H$. The differential rate for the decay of a $M_+$ particle with momentum $p$ into three $M_-$ particles with momenta $p_1, p_3, p_3$ is

$$d\Gamma = 2\pi|V|^2 \delta \left( p - \sum_{j=1}^{3} p_j \right) \delta \left( \omega_+(p) - \sum_{j=1}^{3} \omega_-(p_j) \right) \frac{dp_1 dp_2 dp_3}{3!},$$

where the factor of 3! is introduced to account for the fact that the three particles in the final state are indistinguishable. In the Born approximation the transition matrix element $M$ is

$$M = \frac{1}{4\pi^2} \langle 0 | \prod_{j=1}^{3} c_-(-p_j) V c_+^\dagger(p_j) | 0 \rangle \left( \delta \left( p - \sum_{j=1}^{3} p_j \right) \right)^{-1},$$

$$= \frac{g_3 3!}{2\pi} f(p_1, p_2, p_3).$$

\hspace{1cm} (2.38)
Taking the $M_+$ particle to be at rest, i.e. setting $p = 0$, we obtain
\[ \Gamma = \frac{6g_3^2}{2\pi} \int dp_1 dp_2 |f(p_1, p_2, -p_1 - p_2)|^2 \delta(\omega_+(0) - \omega_-(p_1) - \omega_-(p_2) - \omega_-(p_1 + p_2)) \quad (2.39) \]

In order to simplify matters further, we concentrate on the case where the magnetic field is close to the critical field $H_d$, at which the decay $M_+ \rightarrow M_- M_- M_-$ first becomes kinematically possible. In this regime we have
\[ \omega_+(0) - 3\omega_-(0) \ll \omega_-(0). \quad (2.40) \]

Then the momenta $p_{1,2}$ in (2.39) have to be small in order to satisfy the delta-function and we may use the expansions (2.36) for $f$ and
\[ \omega_-(p) \approx \omega_-(0) + \hat{\alpha} p^2 + \mathcal{O}(p^4), \]
\[ \hat{\alpha} = v^2 \left[ 1 - \frac{H^2}{m\sqrt{H^2 + \Delta^2}} \right] [2\omega_-(0)]^{-1}. \quad (2.41) \]

This leads to the following expression for the decay rate in the regime $H > H_d$,
\[ (H/H_d) - 1 \ll 1 \]
\[ \Gamma \approx \frac{6g_3^2}{2\pi} \hat{C}^2 \frac{4\pi}{(2\hat{\alpha})^4} \sqrt{3} \left[ \omega_+(0) - 3\omega_-(0) \right]^3 \]
\[ \approx g_3^2 \sqrt{3}\hat{C}^2 \left[ \frac{2}{\alpha} \right]^4 \left[ 1 - \frac{\Delta^2}{4m^2} \right]^{3/2} (H - H_d)^3. \quad (2.42) \]

We find that the decay rate is proportional to $(H - H_d)^3$ and is therefore quite small in the vicinity of $H_d$.

3. Landau–Ginzburg (LG) model

A different approach to studying the spin-1 Heisenberg chain with crystal field anisotropies in a magnetic field was used in [10,14]. It is based on the nonlinear sigma model description of the spin-$S$ Heisenberg chain in terms of the three-component field $\vec{\varphi}$ describing the staggered components of the spin operators and the subsequent approximation of replacing the constraint $\varphi^2 = 1$ by a $|\varphi|^4$ interaction. The LG Lagrangian density is [10,14]
\[ \mathcal{L} = \frac{1}{2V} \left( \frac{\partial \vec{\varphi}}{\partial t} + \vec{H} \times \vec{\varphi} \right)^2 - \frac{v}{2} \left( \frac{\partial \vec{\varphi}}{\partial x} \right)^2 - \sum_{a=1}^{3} \frac{\Delta_a^2}{2v} \varphi_a^2 - \lambda |\varphi|^4. \quad (3.1) \]

We again take the magnetic field to point along the three-axis
\[ \vec{H} = H\hat{z}. \quad (3.2) \]

It then follows from (3.1) that $\varphi_3$ couples to the magnetic field only via the $\lambda|\varphi|^4$ interaction. The Landau–Ginzburg theory inherits the discrete symmetries (1.3) and (1.4) from the underlying lattice model. As in the Majorana fermion model it is convenient to combine the translational symmetry by one site $T_R$ with the rotation around the $z$-axis by $\pi R^z_a$ and obtain the following two $Z_2$ symmetries
\[ R^z_a: \quad \varphi_a \longrightarrow -\varphi_a, \quad a = 1, 2 \quad (3.3) \]
\[ T_R R^z_3: \quad \varphi_3 \longrightarrow -\varphi_3. \quad (3.4) \]

The resulting $Z_2 \otimes Z_2$ symmetry is the same as for the Majorana fermion model.
3.1. Spectrum and mode expansion

Neglecting the $|\varphi|^4$ interaction the spectrum can be determined by solving the classical equations of motion

$$
\left[ \frac{\partial^2}{\partial t^2} - v^2 \frac{\partial^2}{\partial x^2} + \Delta^2 - H^2 \right] \varphi_a + 2\epsilon^{abc} H_b \frac{\partial \varphi_c}{\partial t} = 0.
$$

One finds that there are three magnon modes $M_3$ and $M_{\pm}$ with the following dispersion relations

$$
\omega_3(k) = \sqrt{\Delta_3^2 + v^2 k^2},
$$

$$
\omega_{\pm}(k) = \sqrt{H^2 + \frac{\Delta_1^2 + \Delta_2^2}{2} + v^2 k^2} \pm \sqrt{2H^2(\Delta_1^2 + \Delta_2^2 + 2v^2 k^2) + \left( \frac{\Delta_1^2 - \Delta_2^2}{2} \right)^2}.
$$

The low energy $M_-$ mode with dispersion $\omega_-(k)$ becomes gapless at a critical field $H_c = \Delta_1$. The resulting critical point is in the universality class of the two-dimensional Ising model [14].

The scalar fields $\varphi_{1,2}$ have the following mode expansions

$$
\varphi_1(t,x) = \sum_{a=\pm} \int dk \frac{A_{1a}(k)e^{-i\omega_a(k)t+ikx}a_a(k) + h.c.}{\sqrt{4\pi\omega_a(k)/v}},
$$

$$
\varphi_2(t,x) = \sum_{a=\pm} \int dk \frac{iA_{2a}(k)e^{-i\omega_a(k)t+ikx}a_a(k) + h.c.}{\sqrt{4\pi\omega_a(k)/v}},
$$

where $A_{aaa}^*(k) = A_{aaa}(k)$. Here $a$ and $a^\dagger$ obey canonical commutation relations

$$
[a_a(k), a_{\beta}^\dagger(p)] = \delta_{\alpha\beta}\delta(k-p),
$$

and the amplitudes $A_{a\pm}(k)$ are fixed by the requirements that (i) the fields $\varphi_a$ fulfil the equations of motion (3.5) and (ii) the fields $\varphi_a$ and the conjugate momenta $\Pi_a = (1/v)(\partial\varphi_a/\partial t) + (H \times \varphi)_a$ fulfil canonical commutation relations

$$
[\varphi_a(t,x), \varphi_b(t,y)] = 0, \quad [\Pi_a(t,x), \Pi_b(t,y)] = 0, \quad [\varphi_a(t,x), \Pi_b(t,y)] = i\delta_{ab}\delta(x-y).
$$

We find

$$
A_{1+}^2(k) = \frac{3H^2 + \Delta_1^2 + v^2 k^2 - \omega_-(k)^2}{\omega_+(k)^2 - \omega_-(k)^2},
$$

$$
A_{1-}^2(k) = 1 - A_{1+}^2(k) = \frac{\omega_+(k)^2 - 3H^2 - \Delta_1^2 - v^2 k^2}{\omega_+(k)^2 - \omega_-(k)^2},
$$

$$
\frac{A_{2a}(k)}{A_{1a}(k)} = -\frac{\omega_a(k)^2 + H^2 - \Delta_1^2 - v^2 k^2}{2H\omega_a(k)}, \quad a = \pm.
$$

Equations (3.10) allow us to deduce the polarizations of the modes corresponding to the dispersion $\omega_-(k)$. For example, at $H = 0$ the $M_-$ mode is polarized entirely along the
one direction and the $M_+$ mode along the two direction. On the other hand, as $H \rightarrow \Delta_1$ we find that
\[ A_{2-}(0) \rightarrow 0, \quad A_{2+}^2(0) \rightarrow 1, \]
\[ A_{1-}^2(0) \rightarrow \frac{\Delta_3^2 - \Delta_1^2}{3\Delta_5^2 + \Delta_2^2}, \quad A_{1+}^2(0) \rightarrow \frac{4\Delta_3^2}{3\Delta_5^2 + \Delta_2^2}. \] (3.11)
Hence $\varphi_2$ couples only to the $M_+$ mode whereas $\varphi_1$ couples to the $M_+$ mode as well as to the $M_-$ mode with a strength set by the anisotropy.

### 3.2. Decay processes

In the absence of the nonlinear $|\varphi|^4$-term the LG model describes three coherent magnons $M_3, M_\pm$ with corresponding dispersion relations (3.6). Inclusion of the $|\varphi|^4$ term generates interaction terms involving four particles. As was the case in the Majorana fermion model, $\omega_-(k)$ can become very small when the magnetic field is increased and as a result the decays $M_3 \rightarrow M_-M_-M_-$ and $M_+ \rightarrow M_-M_-M_+$ become kinematically allowed. The decay of $M_3$ is forbidden by the symmetry $T_{R}R_{\pi}$ (3.4): $M_3$ is odd under this symmetry whereas $M_\pm$ are even. On the other hand the decay process $M_+ \rightarrow 3M_-$ is allowed when the magnetic field is larger than
\[ H_d = \left[ \frac{17}{16} \left( \Delta_1^2 + \Delta_2^2 \right) \pm \frac{5}{16} \sqrt{13} \left[ \Delta_1^4 + \Delta_2^4 + 10 \Delta_1^2 \Delta_2^2 \right] \right]^{1/2}. \] (3.12)
The interaction describing this decay process is given by
\[ V = \frac{\lambda v^2}{2\pi} \int_{-\infty}^{\infty} \int d^2k_1 \int d^2k_2 \int d^2k_3 g(k_1, k_2, k_3) a_+^\dagger(k_1) a_+^\dagger(k_2) a_+^\dagger(k_3) a_+(k_1 + k_2 + k_3), \] (3.13)
where $g(k_1, k_2, k_3)$ is a symmetric function of its arguments. Its zero momentum limit is
\[ g(0, 0, 0) = \frac{A_{1-}(0)^3 A_{1+}^3(0)}{\omega_-^3 \omega_+} \left[ 1 - \left( \frac{\omega_-^2 + H^2 - \Delta_1^2}{2H \omega_-} \right)^2 \right] \left[ 1 + \frac{\omega_-^2 + H^2 - \Delta_1^2}{2H \omega_-} \frac{\omega_+^2 + H^2 - \Delta_1^2}{2H \omega_+} \right] \]
\[ = \frac{C}{\sqrt{\omega_-^3 \omega_+}}, \] (3.14)
where $\omega_\pm \equiv \omega_\pm(0)$. As a first approximation we neglect all interactions except $V$ and calculate the decay rate $M_+ \rightarrow 3M_-$ in the Born approximation.

The differential rate for the decay of a $M_+$ magnon with momentum $p$ into three $M_-$ magnons with momenta $p_1, p_3, p_3$ is again given by (2.37), where
\[ M = \langle 0 | \prod_{j=1}^{3} a_-(p_j) V a_+^\dagger(p) | 0 \rangle \left( \delta \left( p - \sum_{j=1}^{3} p_j \right) \right)^{-1} \]
\[ = \frac{3\lambda v^2}{\pi} g(p_1, p_2, p_3). \] (3.15)
Taking the $M_+$ magnon to be at rest, i.e. setting $p = 0$, we obtain
\[ \Gamma = \frac{3\lambda v^4}{\pi} \int d^2p_1 \int d^2p_2 \left| g(p_1, p_2, -p_1 - p_2) \right|^2 \delta(\omega_+(0) - \omega_-(p_1) - \omega_-(p_2) - \omega_-(p_1 + p_2)). \] (3.16)
For $H$ slightly larger than $H_d$ we again have
\[ \omega_+(0) - 3\omega_-(0) \ll \omega_-(0), \] (3.17)
and the momenta $p_{1,2}$ in (3.16) have to be small in order to satisfy the delta-function. We may use the expansions (3.14) for $g$ and
\[ \omega_-(p) \approx \omega_-(0) + \alpha p^2 + O(p^4), \]
\[ \alpha = \frac{v^2}{2\omega_-(0)} \left[ 1 - \frac{2H^2}{\sqrt{2H^2(\Delta_1^2 + \Delta_2^2) + ((\Delta_1^2 - \Delta_2^2)/2)^2}} \right]. \] (3.18)
This leads to the following expression for the decay rate in the regime $H > H_d$, $(H/H_d) - 1 \ll 1$
\[ \Gamma \approx \frac{\sqrt{3}\lambda^2 v^4 C^2}{\alpha \omega_-(0)^3 \omega_+(0)}. \] (3.19)
The result (3.19) would suggest that the decay rate switches on suddenly at a finite value as soon as $H$ becomes larger than $H_d$. The underlying reason for this jump is the restricted phase space of a one-dimensional system. The ‘free boson’ result (3.19) for the decay rate is dramatically different from the result obtained in the framework of the Majorana fermion theory. This poses the question whether (3.19) is robust if we take into account interactions among the magnons in the final state. This amounts to resumming the leading infrared divergences in a perturbative expansion in $\lambda$. If we assume that in the low-energy limit the $M_\lambda$ degrees of freedom in the Landau–Ginzburg model can still be mapped onto a Bose gas with $\delta$-function interactions [16], the result of a such a resummation can be determined by exploiting the fact the wavefunctions of the $M_\lambda$ modes reduce to a free fermion form in the limit of small momenta [19]. A three-particle state in the position representation can be written as
\[ |\lambda_1, \lambda_2, \lambda_3 \rangle = \int dx_1 dx_2 dx_3 \chi(x_1, x_2, x_3) a^\dagger_\lambda(x_1) a^\dagger(x_2) a^\dagger(x_3) |0\rangle, \] (3.20)
where the wavefunction is given by
\[ \chi_\lambda(x_1, x_2, x_3) = \frac{(-1)^3}{(2\pi)^3/3!} \prod_{j<k=1}^3 \text{sgn}(x_j - x_k) \sum_{P \in S_3} \text{sgn}(P) e^{\Sigma_{j=1}^3 i \lambda_{Pj} x_j}. \] (3.21)
Here $P$ denotes a permutation of three elements and $S_3$ the symmetric group of degree 3.
In momentum space we have
\[ |\lambda_1, \lambda_2, \lambda_3 \rangle = \int \frac{dk_1 dk_2 dk_3}{(2\pi)^3} \prod_{j=1}^3 \frac{2k_j}{k_j^2 + \epsilon^2} \times a^\dagger_\lambda(\lambda_1 - k_2 - k_3) a^\dagger_\lambda(\lambda_2 - k_1 + k_3) a^\dagger_\lambda(\lambda_3 + k_1 + k_2) |0\rangle. \] (3.22)
Taking (3.22) as the final state, the matrix element of the decay vertex is
\[ M = \frac{\langle \lambda_3, \lambda_2, \lambda_1 | V a^\dagger_\lambda(p) | 0 \rangle}{\delta(p - \sum_{j=1}^3 \lambda_j)} \]
\[ = \frac{3\lambda v^2}{\pi} \int \frac{dq_1 dq_2}{2\pi} \frac{2q_j}{q_j^2 + \epsilon^2} g(\lambda_1 - q_2 - q_3, \lambda_2 - q_1 + q_3, \lambda_3 + q_1 + q_2). \] (3.23)
It follows from the definition (3.23) that the matrix element is an antisymmetric function of \(\lambda_1, \lambda_2, \lambda_3\). As long as we are interested in the decay rate for \(H\) close to \(H_d\), we may expand \(M\) for small \(\lambda_j\). The leading term antisymmetric in \(\lambda_{1,2,3}\) is then
\[
C'(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_3). \tag{3.24}
\]
For small \(\lambda_j\) the matrix element is thus equal to
\[
M = \frac{3\lambda C''v^2}{\pi} \prod_{j<k}(\lambda_j - \lambda_k). \tag{3.25}
\]
Following through the same steps as before, the decay rate for \(H\) close to \(H_d\) with the \(M_+\) magnon initially at rest is found to be
\[
\Gamma \approx \frac{\sqrt{3}\lambda^2 v^4}{4\alpha^4} [\omega_+(0) - 3\omega_-(0)]^3 \propto [H - H_d]^3. \tag{3.26}
\]
Comparing the decay rate (3.26) to the result (3.19) we see that interactions in the final state have a dramatic effect: rather than turning on at a finite value as soon as \(H\) exceeds \(H_d\), the decay rate (3.26) actually vanishes at \(H_d\) and exhibits the same power law behaviour for \(H > H_d\) as the decay rate in the Majorana fermion model. This may suggest that the dependence of the decay rate on \(H - H_d\) is a robust result that holds for the underlying lattice model as well.

4. Vicinity of the Ising critical point

As we have seen above, both the Majorana fermion model and the Landau–Ginzburg theory lead to an Ising critical point at some values \(H_c\) of the applied magnetic field. In the simplest approximations where interactions are neglected, the actual values for \(H_c\) are rather different, but as we are interested only in robust features this numerical difference does not really concern us here. More importantly both theories predict that the low-energy behaviour in the vicinity of the critical point is described by an off-critical Ising model with Hamiltonian
\[
\mathcal{H} = \frac{i v}{2} [L \partial_x L - R \partial_x R] - i m_0 R L. \tag{4.1}
\]
Here the mass parameter that parameterizes the deviation from criticality is equal to the smallest magnon gap
\[
|m_0| \simeq \omega_-(k = 0, H). \tag{4.2}
\]
The description by (4.1) is appropriate at low energies \(\omega \ll \min\{\omega_+(k = 0, H), \omega_3(k = 0, H)\}\) and \(H\) sufficiently smaller than the critical field \(H_{c2}\) (2.22) at which incommensurabilities develop (see figure 1). The Hamiltonian (4.1) exhibits a \(Z_2\) symmetry
\[
R \rightarrow -R, \quad L \rightarrow -L, \tag{4.3}
\]
under which the Ising order (\(\sigma\)) and disorder (\(\mu\)) parameters transform as
\[
H < H_c: \quad \sigma \rightarrow -\sigma, \quad \mu \rightarrow \mu, \quad H > H_c: \quad \sigma \rightarrow \sigma, \quad \mu \rightarrow -\mu. \tag{4.4}
\]
Figure 1. Magnon gaps as functions of the applied field for the Majorana fermion model with $g_a = 0$. The gaps in zero field are chosen as $\Delta_1 = 0.8m$, $\Delta_2 = 1.2m$ and $\Delta_3 = 3.5m$. The square indicates the window in energies and fields in which the description in terms of an effective Ising model is appropriate.

In order to determine the magnetic low-energy response (in the vicinity of the antiferromagnetic wavenumber) we need to express the staggered magnetizations $n^a$ in terms of operators related to the Ising model (4.1). As was pointed out in [14], the dominant contribution to the staggered magnetization in the $x$-direction should be the Ising order parameter field

$$n^x = C_x(H)\sigma + \cdots. \quad (4.5)$$

Here $C_x(H)$ is an unknown constant and the dots indicate contributions from less relevant operators. The underlying reason for the identification (4.5) is simply that in the ordered phase of the Ising model (which corresponds to $H > H_c$) one has a nonzero expectation value $\langle \sigma \rangle \neq 0$, whereas in the disordered phase (which occurs at $H < H_c$) one has $\langle \sigma \rangle = 0$. The staggered magnetization in both the Majorana fermion and LG models exhibits the same kind of behaviour and it is then natural to expect the identification (4.5).

In appendix D we present arguments that suggest that the staggered magnetization along the $y$-direction has the following low-energy projection

$$n^y = C_y(H)\partial_x\sigma + \cdots. \quad (4.6)$$

In what follows we chose a short-distance normalization for the field $\sigma$ in the theory (4.1) such that for $\tau^2 + x^2/v^2 \rightarrow 0$

$$\langle \sigma(\tau,x)\sigma(0,0) \rangle \rightarrow \frac{1}{[\tau^2 + x^2/v^2]^{1/8}}. \quad (4.7)$$

We will use the integrability of the theory (4.1) to determine the dynamical structure factor $S^{xx}(\omega, (\pi/a_0) + q)$ at low energies, where the staggered component of $S^x$ is given by (4.5). The $yy$ component then follows from (4.6)

$$S^{yy}(\omega, \frac{\pi}{a_0} + q) \propto \frac{\omega^2}{m^2}S^{xx}(\omega, \frac{\pi}{a_0} + q). \quad (4.8)$$
4.1. \( H < H_c \): low-field phase

By the \( Z_2 \) symmetry (4.3), (4.4) only intermediate states with an odd number of magnons contribute to the two-point correlation functions of the Ising order parameter field \( \sigma \) and hence the staggered structure factor \( S^{xx}(\omega, (\pi/a_0) + q) \) at low energies. The leading contributions are [20]–[23]

\[
S^{xx}(\omega, \frac{\pi}{a_0} + q) = \frac{vA}{\sqrt{m_0^2 + v^2q^2}} \delta \left( \omega - \sqrt{m_0^2 + v^2q^2} \right) + \frac{2vA}{3\pi^2m_0^2} \int_{z_0}^{\infty} dz \frac{(\tanh(z) \tanh((y+z)/2) \tanh((y-z)/2))^2}{\sqrt{x^2 - 4 \cosh^2 z - 16 \cosh^2 z}}
\]

+ contributions from 5, 7, \ldots magnons, \hspace{1cm} (4.9)

where

\[
A = C_x^2(H)2^{1/6}e^{-1/4}A^3m_0^{1/4},
\]

\[
x^2 = \frac{\omega^2 - v^2q^2}{m_0^2},
\]

\[
z_0 = \text{arccosh} \left( \frac{x - 1}{2} \right),
\]

\[
y = \text{arccosh} \left( \frac{x^2 - 1 - 4 \cosh^2 z}{4 \cosh z} \right). \hspace{1cm} (4.11)
\]

Here

\[
A = 1.28242712910062\ldots \hspace{1cm} (4.12)
\]

is Glaisher's constant. The three-magnon contribution is always very small. In the frequency interval \([0, 30m_0]\) roughly 100 times more spectral weight sits in the single-magnon contribution than in the three-particle one. Hence the magnetic response below energies of the order of tens of the magnon gap \( m_0 \) is dominated by the coherent magnon contribution. However, if \( H \) becomes very close to \( H_c \) the magnon gap \( m_0 \) tends to zero. If we are interested in the magnetic response at a low (compared to the gap of the second coherent magnon mode) but fixed energy we have to take the contributions of intermediate states with 5, 7, 9, \ldots magnons into account in order to get an accurate result for \( S^{xx}(\omega, (\pi/a_0) + q) \).

4.2. \( H = H_c \): at criticality

At criticality the structure factor exhibits a power-law behaviour [24]

\[
S^{xx}(\omega, \frac{\pi}{a_0} + q) = \text{Im}\{B[v^2q^2 - (\omega + i\varepsilon)^2]^{-7/8}\}, \hspace{1cm} (4.13)
\]

where

\[
B = 2vC_x^2(H)2^{3/4} \frac{\Gamma(7/8)}{\Gamma(1/8)}. \hspace{1cm} (4.14)
\]
4.3. $H > H_c$: high-field phase

In this phase there is a nonzero staggered magnetization and correspondingly a nonzero expectation value for the Ising order parameter

$$\langle \sigma \rangle \neq 0,$$

which results in a Bragg peak for momentum transfer $\pi/a_0$ along the chain direction. By virtue of the $Z_2$ symmetry (4.4) only intermediate states with an even number of magnons contribute to $S_{xx}^\pm (\omega, (\pi/a_0)+q)$. The leading contribution to the inelastic neutron scattering cross section comes from intermediate states involving two magnons [20]–[22], which leads to the following result

$$S_{xx}^\pm (\omega, \frac{\pi}{a_0} + q) = \frac{vA}{\pi} \sqrt{s^2 - 4m_0^2} \theta(s - 2m_0) + \text{contributions from 4, 6, \ldots magnons}.$$  

(4.16)

Here $A$ is given by (4.10) and $s^2 = \omega^2 - v^2 q^2$.

5. The high-field phase for weak anisotropy

In general it is difficult to determine the effects of magnon-interactions in quantitative detail. An exception is the case of a small anisotropy of the zero-field gaps

$$\Delta \ll m,$$

where $2m = \Delta_1 + \Delta_2$ and $2\Delta = \Delta_2 - \Delta_1$. As we will show, if the magnetic field is sufficiently larger than the critical field $H_c$ and

$$\Delta \ll H - H_c \lesssim J,$$

it is possible to determine the interaction effects on the magnetic response at low energies in some detail. More precisely, we consider magnetic fields sufficiently larger than the field $H_{c2}$ (see e.g. (2.22)), at which incommensurabilities begin to develop. The scale defining the low-energy region is the difference $\Delta$. As is shown in appendix E, the low-energy effective Hamiltonian is given by a sine-Gordon model (SGM) [14]

$$H = \frac{\tilde{v}}{16\pi} \left[ (\partial_x \Theta)^2 + (\partial_x \Phi)^2 \right] - 2\mu \cos \beta \Theta.$$  

(5.3)

Here $\tilde{v}$ is the spin velocity, $\mu \propto \Delta$ and $\beta$ is a function of the applied magnetic field $H$. The high-energy cutoff of the theory (5.3) is $H - H_c$. At low energies the dominant Fourier component of the transverse spin operators is at $q = \pi/a_0$

$$S_j^\pm \rightarrow (-1)^j A \exp \left( \pm \frac{i\beta}{2} \Theta \right).$$

(5.4)

The identification (5.4) is in accordance with the fact that in the high-field phase there is Néel order along the $x$-direction

$$\langle (-1)^n S_n^x \rangle \propto \left\langle \cos \left( \frac{\beta}{2} \Theta \right) \right\rangle \neq 0.$$  

(5.5)
Haldane-gap chains in a magnetic field

Figure 2. Parameter $\beta$ as a function of the applied magnetic field.

We choose a short-distance normalization such that for $|x - y| \to 0$
$$e^{i\alpha \Theta(x)} e^{i\gamma \Theta(y)} \to |x - y|^{-\alpha \gamma} e^{i\alpha \Theta(x) + i\gamma \Theta(y)}. \hspace{1cm} (5.6)$$

The amplitude $A$ in (5.4) is nonuniversal and not known in general. However, very close to $H_c$,
$$\Delta \ll H - H_c \ll H_c, \hspace{1cm} (5.7)$$
it is given by (see appendix F)
$$A = A' \left[ \frac{a_0^2 m}{v^2} (H - H_c) \right]^{1/8}, \hspace{1cm} (5.8)$$
where $A'$ is a field independent numerical constant. The dependence of (5.8) on $H - H_c$ is a universal feature of the C–IC transition.

We note that the sign of the cos-term in (5.3) is quite important. Flipping the sign corresponds to a shift $\Theta \to \Theta + \pi/\beta$, which essentially leads to an exchange of the $x$ and $y$ component of the spin operators in (5.4).

The value of the parameter $\beta$ is of crucial importance. For the isotropic case ($\Delta_2 = \Delta_1$) it has recently been determined [13] in the framework of the nonlinear sigma model description of the spin-$S$ Heisenberg chain. In the isotropic case the high-field phase at $H > H_c$ is a Luttinger liquid and $\beta$ is related to the Luttinger liquid parameter. It was found that [13]
$$\beta = \frac{1}{\sqrt{2S_R(\theta_F)}}, \hspace{1cm} (5.9)$$
where $S_R(\theta)$ fulfils the integral equation
$$S_R(\theta) = 1 + \int_{-\theta_F}^{\theta_F} d\theta' S_R(\theta') \frac{1}{\pi^2 + (\theta - \theta')^2}. \hspace{1cm} (5.10)$$
Here $\theta_F$ is determined as a function of the magnetic field $H$ by

$$\epsilon(\theta) = m \cosh(\theta) - H + \int_{-\theta_F}^{\theta_F} d\theta' \frac{\epsilon(\theta')}{\pi^2 + (\theta - \theta')^2},$$

$$\epsilon(\theta_F) = 0.$$  

(5.11)

Similarly one may determine the spin velocity

$$\tilde{v} = \frac{v}{2\pi \rho(\theta)} \frac{\partial \epsilon(\theta)}{\partial \theta} \bigg|_{\theta = \theta_F},$$

(5.12)

where $\rho(\theta)$ fulfills the integral equation

$$\rho(\theta) = \frac{m}{2\pi} \cosh(\theta) + \int_{-\theta_F}^{\theta_F} \frac{\rho(\theta')}{\pi^2 + (\theta - \theta')^2}.$$  

(5.13)

The parameter $\beta$ as well as the velocity $\tilde{v}$ entering the sine-Gordon Hamiltonian (5.3) may be estimated with a good degree of accuracy from their respective values in the isotropic case as long as $(\Delta_2 - \Delta_1)/\Delta_2 \ll 1$. On the other hand, the agreement between the Luttinger liquid parameter calculated in the nonlinear sigma model and the one of the isotropic spin-1 Heisenberg chain in a magnetic field, which is known approximately from DMRG computations [17], was shown to be fairly good in [13]. Hence we may determine $\beta$ with a reasonable degree of accuracy from (5.9) as long $(\Delta_2 - \Delta_1)/\Delta_2 \ll 1$. It then follows that $\beta < 1/\sqrt{2}$ and hence the SGM (5.3) is in the attractive regime.

5.1. Spectrum of the SGM

The SGM (5.3) is integrable and many exact results are available. The spectrum of the SGM depends on the value of the coupling constant $\beta$. In the so-called repulsive regime, $1/\sqrt{2} < \beta < 1$, there are only two elementary excitations, called soliton and antisoliton. These have a massive relativistic dispersion,

$$E(P) = \sqrt{M^2 + \tilde{v}^2 P^2},$$

(5.14)

where $M$ is the gap.

In the regime $0 < \beta < 1/\sqrt{2}$ relevant to our discussion, soliton and antisoliton attract and can form bound states known as ‘breathers’. There are different types of breather, where $[x]$ in (5.15) denotes the integer part of $x$. The breather gaps are given by

$$M_n = 2M \sin(n\pi \xi/2), \quad n = 1, \ldots, \mathcal{N},$$

(5.16)

where

$$\xi = \frac{\beta^2}{1 - \beta^2}.$$  

(5.17)
The number of breathers is a function of the applied magnetic field \( H \). There is always at least one breather. A second breather appears above a field \( H_0 \), which is determined by the requirement

\[
\beta = \frac{1}{\sqrt{3}}. \tag{5.18}
\]

This requirement is fulfilled for

\[
H > H_0 \approx 1.5 M. \tag{5.19}
\]

### 5.2. Dynamical structure factor

A basis of eigenstates of the SGM is given by scattering states of solitons, antisolitons and breathers. In order to distinguish these we introduce labels \( B_1, B_2, \ldots, B_N, s, \bar{s} \). As usual for particles with relativistic dispersion, it is useful to introduce a rapidity variable \( \theta \) to parameterize energy and momentum

\[
E_s(\theta) = M \cosh \theta, \quad P_s(\theta) = (M/\tilde{v}) \sinh \theta, \tag{5.20}
\]

\[
E_{\bar{s}}(\theta) = M \cosh \theta, \quad P_{\bar{s}}(\theta) = (M/\tilde{v}) \sinh \theta, \tag{5.21}
\]

\[
E_{B_n}(\theta) = M_n \cosh \theta, \quad P_{B_n}(\theta) = (M_n/\tilde{v}) \sinh \theta. \tag{5.22}
\]

Two-point functions are expressed in terms of a basis of scattering states of solitons, antisolitons and breathers as summarized in appendix B, see equation (B.8). After carrying out the double Fourier transform we arrive at the following representation for the imaginary part of the retarded two-point function of the operator \( \mathcal{O} \) for \( \omega > 0 \)

\[
S^\mathcal{O}(\omega, q) = \sum_{n=1}^{\infty} \sum_{\epsilon} \int \frac{d\theta_1, \ldots, d\theta_n}{(2\pi)^n} |f_{\epsilon_1, \ldots, \epsilon_n}(\theta_1, \ldots, \theta_n)|^2 \times \delta \left( q - \sum_j M_{\epsilon_j} \sinh \theta_j/\tilde{v} \right) \delta \left( \omega - \sum_j M_{\epsilon_j} \cosh \theta_j \right). \tag{5.23}
\]

The form factors of the operators \( \exp(\pm i\beta \Theta/2) \) in the sine-Gordon model were determined in [28, 29]. Using these results we can determine the first few terms of the expansion (5.23) for the transverse spin operators. We have \((s^2 = \omega^2 - v^2 q^2)\)

\[
S^{xx}(\omega, \pi a_0 + q) = C \left\{ \pi f_2 \delta(s^2 - M_2^2) \Theta(H - H_0) + \text{Re} \frac{|F^{\cos}(\theta_0)|^2}{s\sqrt{s^2 - 4M^2}} + \cdots \right\}, \tag{5.24}
\]

\[
S^{yy}(\omega, \pi a_0 + q) = C \left\{ \pi f_1 \delta(s^2 - M_1^2) + \text{Re} \frac{|F^{\sin}(\theta_0)|^2}{s\sqrt{s^2 - 4M^2}} + \cdots \right\}.
\]

Here \( C \) is an overall (dimensionful) constant. The terms proportional to \( F^{\sin} \) and \( F^{\cos} \) represent the contributions by intermediate states involving one soliton and one antisoliton and

\[
\theta_0 = 2 \text{arccosh}(s/2M). \tag{5.25}
\]
Haldane-gap chains in a magnetic field

The $\delta$-function contributions are due to the breather bound states. The soliton–antisoliton form factors are given by \cite{28,29}

\[
|F^{\sin}(\theta)|^2 = \langle 0 | \sin \left( \frac{\beta}{2} \Phi(0) \right) | \theta_2 \theta_1 \rangle_{+-}^2 = \frac{g(\theta)}{\xi \cosh \left( (\theta + i\pi)/2\xi \right)}^2, \\
|F^{\cos}(\theta)|^2 = \langle 0 | \cos \left( \frac{\beta}{2} \Phi(0) \right) | \theta_2 \theta_1 \rangle_{+-}^2 = \frac{g(\theta)}{\xi \sinh \left( (\theta + i\pi)/2\xi \right)}^2,
\]

where $\theta = \theta_2 - \theta_1$ and

\[
g(\theta) = i \sinh \theta/2 \exp \left( \int_0^\infty \frac{dt}{t} \frac{\sinh^2(t(1 - i\theta/\pi)) \sinh(t[\xi - 1])}{\sinh 2t \sinh \xi t \cosh t} \right). \tag{5.27}
\]

The absolute values squared of the breather form factors are \cite{28,29}

\[
f_1 = 2 \sin \left( \frac{\pi \xi}{2} \right) \exp \left( -2 \int_0^\pi \frac{dt}{2\pi} \frac{t}{\sin t} \right), \\
f_2 = \frac{2|g(-i\pi[1 - 2\xi])|^2}{\cot(\pi \xi) \cot(\pi \xi/2)^2}. \tag{5.28}
\]

An important result is that the first bound state $B_1$ is visible only in $S^{yy}$ and does not couple to $S^{xx}$. We note that there are additional contributions in the spectral representations (5.24) at higher energies. For example, there is a two-breather $B_1B_1$ contribution to $S^{xx}$ at energies above $2M_1$.

We plot $S^{xx}(\omega, \pi/a_0)$ as functions of $\omega/M$ for several values of the applied magnetic field in figures 3 and 4. In order to give a visual impression of their spectral weights we have broadened the $\delta$-functions corresponding to the breathers by convolution with a Gaussian.

We first discuss the evolution of $S^{yy}(\omega, \pi/a_0)$ shown in figure 3: as $H$ moves away from $H_c = m$ the breather $B_1$ splits off from the soliton–antisoliton continuum and very quickly takes over most of the spectral weight. Except for a narrow window (in magnetic field) above $H_c$ the $yy$-component of the dynamical structure factor is dominated by a coherent single-particle peak.

The evolution of $S^{xx}(\omega, \pi/a_0)$ is very different, as is shown in figure 4: as $H$ moves away from $H_c = m$ the incoherent soliton–antisoliton continuum slowly narrows (on the scale of the field-dependent soliton gap) until it eventually begets the second heavy breather $B_2$ at $H = H_0 \approx 1.5m$. Over a large interval of magnetic fields $S^{xx}(\omega, \pi/a_0)$ is dominated by the incoherent soliton–antisoliton continuum.

5.2.1. Spectral weights. In order to compare the spectral weights located in the coherent breather peaks to the spectral weight associated with the soliton–antisoliton continua it is useful to define quantities

\[
I^{xx} = \frac{M^2}{C} \int_0^{25} dx \ S^{xx} \left( xM, \frac{\pi}{a_0} \right) \equiv I^{xx}_{B_2} + I^{xx}_{ss}, \\
I^{yy} = \frac{M^2}{C} \int_0^{25} dx \ S^{yy} \left( xM, \frac{\pi}{a_0} \right) \equiv I^{yy}_{B_1} + I^{yy}_{ss}. \tag{5.29}
\]

J. Stat. Mech.: Theor. Exp. (2004) P12006 (stacks.iop.org/JSTAT/2004/P12006)
For example, \(C I_{yy}^y M^2\) is the spectral weight of the \(yy\)-component of the dynamical structure factor at the antiferromagnetic wavenumber integrated over the frequency interval \([0, 25M]\). It has contributions \(I_{yy}^{yB_1}\) from the coherent breather peak and \(I_{yy}^{yss}\) from the soliton antisoliton continuum (there are also contributions due to \(B_1B_2\) two-breather states, etc, but their contributions are subleading). It is important to note that the soliton gap \(M\) and the overall factor \(C\) depend on the applied magnetic field. These dependencies drop out once we consider spectral weight ratios such as

\[
\frac{I_{yy}^{yss}}{I_{yy}^{yB_1}}, \quad \frac{I_{xx}^{xx}}{I_{yy}^{yB_1}}, \quad \frac{I_{xx}^{xx}}{I_{yy}^{yB_1}}.
\]

These ratios are plotted as functions of \(\beta\) in figure 5. We see that for small \(\beta\) (that is at \(H \gg H_c\)) most of the spectral weight is situated in the coherent peak associated with the first breather \(B_1\). Very close to the transition the second breather does not exist and most of the spectral weight sits in the soliton–antisoliton continua. The crossover between these two regimes occurs around \(\beta \approx 0.675\), which according to figure 2 corresponds to

\[
\frac{H}{H_c} \approx 1.025.
\]

The lesson is that interactions make the summed dynamical structure factor

\[
S^{xx}(\omega, \pi/a_0 + q) + S^{yy}(\omega, \pi/a_0 + q)
\]
Figure 4. $S^{xx}(\omega, \pi/a_0)$ as a function of $\omega/M$ for several values of the applied field $H$.

look coherent except for fields very close to $H_c$. On the other hand, the polarized structure factor $S^{xx}(\omega, (\pi/a_0) + q)$ looks incoherent! It would be very interesting to attempt to disentangle the components of the dynamical structure factor in inelastic neutron scattering experiments and in this way observe this incoherent scattering continuum.

5.2.2. Polarizations in the LG model. How do these results fit into the general picture of the LG model? In the latter one expands to quadratic order in the fields $\varphi_1$ and $\varphi_2$ around the minimum of the effective potential at $\vec{\varphi}_{\text{vac}} = (m_0, 0, 0)$

$$m_0^2 = \frac{H^2 - \Delta_2^2}{4v\lambda}.$$ \hfill (5.33)

The effective Lagrangian for the fields $\varphi_{1,2}$ becomes

$$\mathcal{L} = \sum_{a=1}^{2} \frac{1}{2v} \left( \frac{\partial \varphi_a}{\partial t} \right)^2 - \frac{v}{2} \left( \frac{\partial \varphi_a}{\partial x} \right)^2 - \frac{H_c}{v} \epsilon_{abc} \frac{\partial \varphi_a}{\partial t} \varphi_b - \frac{H^2 - \Delta_1^2}{v} \varphi_1^2 - \frac{\Delta_2^2 - \Delta_1^2}{2v} \varphi_2^2.$$ \hfill (5.34)

This is the same as (3.1) for the fields $\varphi_{1,2}$ if we make the replacement (in (3.1))

$$\Delta_1^2 \rightarrow 3H^2 - 2\Delta_1^2, \quad \Delta_2^2 \rightarrow \Delta_2^2 + H^2 - \Delta_1^2.$$ \hfill (5.35)

This implies for the polarizations in the limit $H \gg \Delta_2$

$$\frac{A_{2, \omega}(0)}{A_{1, \omega}(0)} \rightarrow \left[ \frac{3H^2}{\Delta_2^2 - \Delta_1^2} \right]^{1/2}.$$ \hfill (5.36)
In other words

$$|A_{2-}| \gg |A_{1-}|,$$  \hspace{1cm} (5.37)

and as a result the coherent low-energy mode is dominantly polarized along the $y$-direction! This agrees nicely with the sine-Gordon calculation, where the dominant feature, the first breather, appears in $S^{yy}$.

6. Interchain coupling

So far we have considered a purely one-dimensional situation corresponding to an ensemble of uncoupled spin-1 chains. As long as the magnon gap is large, a weak coupling between the chains may be neglected in a first approximation. On the other hand, the interchain exchange is expected to lead to significant qualitative changes in the magnetic response close to the critical point where the magnon gap becomes very small [35]. In order to assess the effects of a weak interchain coupling for $H \approx H_c$ we consider a Landau–Ginzburg model of the form

$$\mathcal{L} = \sum_n \mathcal{L}_n + \mathcal{L}_{\text{int}},$$  \hspace{1cm} (6.1)

where

$$\mathcal{L}_n = \frac{1}{2v} \left( \frac{\partial \bar{\varphi}_n}{\partial t} + \vec{H} \times \bar{\varphi}_n \right)^2 - \frac{v}{2} \left( \frac{\partial \bar{\varphi}_n}{\partial x} \right)^2 - \sum_{a=1}^{3} \frac{\Delta^2_a}{2v} \varphi_n^2 - \lambda |\bar{\varphi}_n|^4,$$

$$\mathcal{L}_{\text{int}} = \frac{J_1}{a_0} \sum_{(j,k)} \bar{\varphi}_j \cdot \bar{\varphi}_k.$$  \hspace{1cm} (6.2)
Here the sum $\langle jk \rangle$ is over links between neighbouring sites on different chains and we have dropped quartic terms in $L_{\text{int}}$ that arise from the interaction of the smooth components of the spin operators.

As we have seen in section 4, close to the Ising critical point the low-energy degrees of freedom are described by off-critical Ising models. Hence at low energies we have

$$L_n \approx R_n \partial_- R_n + L_n \partial_+ L_n - i m_0 R_n L_n.$$  \hspace{1cm} (6.3)

The leading low-energy projection of the interchain exchange follows from (4.5), (4.6)

$$L_{\text{int}} \approx \frac{J_{\perp}}{a_0} C^2 \left[ \frac{a_0}{v} \right]^{1/4} \sum_{\langle jk \rangle} \sigma_j \sigma_k,$$  \hspace{1cm} (6.4)

where $C$ is a dimensionless constant. The ‘quasi-1D Ising model’ (6.3), (6.4) has recently been studied in [36] and we may follow some of this analysis here.

**6.1. Mean-field approximation**

As a first step, we analyse the model (6.3), (6.4) by means of a self-consistent mean-field approximation [30,31]. We assume the existence of a nonzero expectation value

$$\langle \sigma \rangle \neq 0,$$  \hspace{1cm} (6.5)

which corresponds to Néel order along the $x$-direction. The long-range order can be induced by the magnetic field, the interchain coupling or by both. In the presence of a nonzero expectation value (6.5) we may decouple the interaction term in (6.4) and arrive at the following mean-field Lagrangian density

$$L_{\text{MF}} = R \partial_- R + L \partial_+ L - i m_0 RL + \frac{h}{v} \sigma.$$  \hspace{1cm} (6.6)

Here ‘magnetic field’ $h$ has dimensions of $s^{-15/8}$ by virtue of the normalization (4.7) and is subject to the self-consistency condition

$$h = Z C^2 \frac{J_{\perp}}{a_0} \left[ \frac{a_0}{v} \right]^{1/4} \langle \sigma \rangle,$$  \hspace{1cm} (6.7)

where $Z$ is the number of neighbouring chains. The mean-field theory is purely one-dimensional and describes an off-critical Ising model in an effective magnetic field induced by the neighbouring chains. The model (6.6) has been studied by several authors [32]–[34] and is known to exhibit very interesting physical behaviour as $m_0$ and $h$ are varied. In order to discuss the effects of $h$ and $m_0$ it is convenient to consider the Euclidean two-point function of Ising order parameters

$$\chi^E_{\sigma \sigma}(\bar{\omega}, q) = \int_{-\infty}^\infty \int_{-\infty}^\infty dx \, d \tau \, e^{i \bar{\omega} \tau - i q x} \langle \sigma(\tau, x) \sigma(0, 0) \rangle.$$  \hspace{1cm} (6.8)

We note that $\chi^E_{\sigma \sigma}$ is related to the $xx$-component of the staggered susceptibility by analytic continuation to real frequencies. The Lagrangian (6.6) defines a one-parameter family of field theories labelled by the dimensionless quantity [34]

$$\chi = m_0 h^{-8/15}.$$  \hspace{1cm} (6.9)

In the two special cases $\chi = 0$ and $|\chi| = \infty$ the model (6.6) is integrable and the susceptibility (6.8) can be determined to a very high accuracy by means of the form factor bootstrap approach. In what follows we first review known quantitative results for the cases $|\chi| \to \infty$ and $\chi \to 0$ and then summarize the qualitative behaviour for general values of $\chi$.  

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J. Stat. Mech.: Theor. Exp. (2004) P12006 (stacks.iop.org/JSTAT/2004/P12006)
6.1.1. The limit \( h \to 0 \): McCoy–Wu scenario. The regime \( h \to 0 \) was studied in \([32, 33]\) by means of a perturbative expansion in \( h \). In the absence of a field \( (h = 0) \) the dynamical structure factor has been given in section 4. For \( m_0 > 0 \) the Ising model is in its disordered phase and the spin–spin correlation functions are dominated by a single-particle pole and the next-lowest excited states occur in the form of a three-particle scattering continuum. The dynamical structure factor is proportional to (4.9). Introducing a small magnetic field leads to a small shift in the position of the single-particle pole. Furthermore a two-particle scattering continuum of excited states emerges.

For \( m_0 < 0 \) the Ising model is in its ordered phase. This means that there is a nonzero value for the staggered magnetization

\[
\langle \sigma \rangle_0^2 = 2^{1/6} e^{-1/4} A^3 m_0^{1/4},
\]

where \( A \) denotes Glaisher’s constant (4.12). The structure factor in the ordered phase is given by (4.16): the structure factor is incoherent and there is a two-particle branch cut starting at \( \omega = 2m_0 \).

It is convenient to define a dimensionless magnetic field \( \tilde{h} \) by

\[
\tilde{h} = \frac{\langle \sigma \rangle_0}{m_0^2} h.
\]

After a resummation of a perturbative expansion in \( \tilde{h} \) McCoy and Wu established that the spin–spin correlation function has the following large-distance behaviour \([32]\)

\[
\langle \sigma(\tau, x) \sigma(0, 0) \rangle \approx \langle \sigma \rangle_0^2 \exp\left(-\frac{2m_0 r}{2 \sqrt{\pi m_0 r}}\right) \tilde{h} \sum_l \exp\left(-m_0 r (\lambda_l \tilde{h}^{2/3})^2\right),
\]

where \( r^2 = \tau^2 + x^2/v^2 \) and \( \lambda_l \) are the positive solutions to the equation

\[
J_{1/3}(\lambda_l/3) + J_{-1/3}(\lambda_l/3) = 0.
\]

The interesting point is that the Fourier transform of (6.12) no longer has a branch cut! There are single-particle poles at

\[
\tilde{\omega}^2 + v^2 q^2 = -[2 + (\tilde{h} \lambda_l)^{2/3}]^2 m_0^2.
\]

In other words, the two-particle branch cut has disintegrated into a series of single-particle poles. The residues of these poles are proportional to

\[
\tilde{h} [2 + (\tilde{h} \lambda_l)^{2/3}]^{-1}.
\]

Hence the lightest particle carries more spectral weight than the heavier ones. This is quite different from the result for \( h = 0 \) where the structure factor vanishes as the threshold is approached from above.
Haldane-gap chains in a magnetic field

6.1.2. The limit \( m_0 \to 0 \): magnetic deformation. In the limit \( m_0 \to 0 \) the model (6.6) is integrable [37]. The spectrum consists of eight types of massive self-conjugate particles. Three of them have masses below the lowest two-particle threshold. The two-point function of the Ising order operator \( \sigma \) was calculated by the form factor bootstrap approach in [38]. The dominant contribution to the two point function of Ising order parameter fields is due to the lightest particles. The dynamical susceptibility is approximately

\[
\chi_{\sigma\sigma}(\omega, q) \approx \left[ \frac{4m_1^2}{15\pi h} \right]^2 \sum_{j=1}^{3} \frac{2vZ_j}{\omega^2 - v^2q^2 - m_j^2},
\]

(6.16)

where the particle masses are [37, 42]

\[
m_1 \approx 4.40490858h^{8/15}, \quad m_2 \approx 1.618m_1, \quad m_3 \approx 1.989m_1
\]

(6.17)

and [36, 38]

\[
Z_1 \approx 0.247159, \quad Z_2 \approx 0.069017, \quad Z_3 \approx 0.02096.
\]

(6.18)

The expectation value of the Ising order parameter is [42]

\[
\langle \sigma \rangle \approx 1.07496h^{1/15},
\]

(6.19)

which enables us in principle to solve the self-consistency equation (6.7). The important point is that most of the spectral weight is located in the coherent modes corresponding to the two lightest particles. The ratio of weights between them is

\[
\frac{(Z_1/m_1)}{(Z_2/m_2)} \approx 5.79427.
\]

(6.20)

The region \( m_0 \approx 0 \) limit was studied by form factor perturbation theory in [34].

6.1.3. Qualitative behaviour in the general case. For general values of \( \chi \) the qualitative behaviour of \( \chi_{\sigma\sigma}^E(\bar{\omega}, q) \) is known and may be conveniently summarized [32, 34] by considering the evolution of \( \chi_{\sigma\sigma}^E \) with \( \chi \) along a path in the \( m_0-h \) plane as shown in figure 6.

In figure 7 we show the analytic structure of \( \chi_{\sigma\sigma}^E \) as a function of \( s = \sqrt{\bar{\omega}^2 + v^2q^2} \) for various locations along the path set out in figure 6. For example, point (a) corresponds to the disordered phase of the off-critical Ising model, where in Euclidean space there is a single-particle pole at \( s = im_0 \) and a three-particle branch cut along the positive imaginary axis starting at \( s = 3im_0 \). Point (b) shows the small shift in the position of the pole and the emergence of a two-particle branchcut [32]. Points (c)–(e) describe the vicinity of the Ising model in a magnetic field; there are several single-particle poles below a two-particle branchcut and the number of these poles increases as we move along the path. Finally, points (f) and (g) describe the breakup of the two-particle branchcut mentioned above.

An important point is that for \( m_0 < 0 \), which corresponds to the ordered phase of the Ising model for \( h = 0 \), the general effect of the magnetic field is to make the dynamical susceptibility look more coherent in these sense that the low-energy regime is dominated by single-particle poles. In particular, a weak interchain coupling in the ordered phase close to \( H_c \) leads to a disintegration of the two-particle scattering continuum that dominates the dynamical structure factor (4.16) and the formation of a series of single-particle poles.
6.2. Beyond mean-field: RPA

It is straightforward to go beyond the mean-field approximation by resumming all diagrams in the interchain coupling that do not involve loops. This leads to the RPA expression for the dynamical susceptibility [39]

\[
\chi^{xx}(\omega, q, k) = \frac{\chi^{xx}(\omega, q)}{1 - 2J_{\perp}(k)\chi^{xx}(\omega, q)},
\]

(6.21)

where \(J_{\perp}(k)\) is the Fourier transform of the interchain coupling and

\[
\chi^{xx}(\omega, q) = \frac{C^2}{a_0} \left[ \frac{a_0}{v} \right]^{1/4} \chi_{\sigma\sigma}(\omega, q).
\]

(6.22)

Figure 6. Path in the \(h-m_0\) plane of the transverse Ising model in a magnetic field.

Figure 7. Structure of poles and branch cuts of \(\chi^{E}_{\sigma\sigma}(\bar{\omega}, q)\) at the points (a)–(g) in the \(h-m_0\) plane indicated in figure 6 (\(m_1 = m_0(2 + (\tilde{h}\lambda_1)^{2/3})\)).
In our notations

\[ J_\perp(k) = J_\perp[\cos(k_y a_0) + \cos(k_z a_0)] \]  

(6.23)

for a simple cubic lattice. It was shown in [36] that in the vicinity of points (c)–(e) of figure 6 the RPA leads only to slight changes of the mean-field results. More precisely, single-particle excitations corresponding to poles at \( s = m \) (with residue \( Z/2m \)) in the 1D susceptibility \( \chi^{xx}(\omega,q) \) acquire a transverse dispersion \( Z J_\perp(k) \) in the RPA.

7. Summary and discussion

We have studied the spectrum and dynamical spin correlations for Haldane-gap systems in the presence of a magnetic field. We have paid particular attention to the role played by the crystal field anisotropies present in materials like NDMAP. We have concentrated on the case where the magnetic field is applied along the same direction as the largest single-ion anisotropy \( D \) (which we identify with the \( z \)-direction in spin space). Generalizations of our results to other cases is straightforward. Our main results are as follows:

- At low fields there are three coherent modes \( M_-, M_+ \) and \( M_3 \). Their respective gaps \( \Delta_-(H) < \Delta_+(H) < \Delta_3(H) \) are field-dependent.
- Above a critical field \( H_d \), \( M_2 \) develops a finite lifetime via the decay process \( M_+ \rightarrow M_- M_- M_- M_- \) and \( M_3 \) retain infinite lifetimes.
- At a critical field \( H_c > H_d \) the gap \( \Delta_-(H) \) vanishes. In the vicinity of \( H_c \) the low energy degrees of freedom are described by an (off-critical) Ising model and the dynamical structure factor is calculated by exact methods. For \( H > H_c \) the dynamical structure factor is dominated by an incoherent two-particle scattering continuum above a finite-energy threshold.
- At fields sufficiently above \( H_c \) the low-energy degrees of freedom are described by a sine-Gordon model. \( S^{yy}(\omega, (\pi/a_0) + q) \) is dominated by a coherent single-particle bound state with a spectral gap below a two-particle scattering continuum. The most pronounced feature in \( S^{xx}(\omega, (\pi/a_0) + q) \) is an incoherent two-particle scattering continuum above a finite-energy threshold.
- The effects of interchain coupling are most pronounced in the vicinity of \( H_c \). Taking it into account in a mean-field fashion leads to a purely one-dimensional effective description at low energies in terms of an Ising model in a magnetic field. This suggests that Haldane-gap materials with single-ion anisotropies in a magnetic field may constitute a realization of this very interesting theory. Within the mean-field description the main effect of interchain coupling is to generate coherent single-particle modes from the incoherent scattering continua. As a result the dynamical structure factor will appear more ‘coherent’.

Our findings shed some light on the question why recent inelastic neutron scattering experiments on NDMAP [4, 5] have failed to find any evidence of scattering continua in the high-field phase. At large fields these are suppressed through bound-state formation, whereas in the vicinity of the critical field \( H_c \) the coupling between chains affects similar shifts of spectral weight to single-particle modes. It would be interesting to investigate some of our predictions experimentally. In particular we hope that it may be possible to:
(1) Address the issue of the finite lifetime of $M_2$ above the critical field $H_d$.

(2) Disentangle the $xx$ and $yy$ components of the structure factor at high fields. According to our predictions the $xx$-component will remain incoherent up to fairly large fields so that a scattering continuum may be observable.

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**Appendix A: Low-field phase in the absence of crystal field anisotropy**

In the absence of crystal field anisotropy the Hamiltonian is

$$\mathcal{H}(h) = J \sum_n S_n \cdot S_{n+1} - h S^z. \quad (A.1)$$

The Heisenberg equations of motion read

$$\frac{d}{dt} S^\pm_n(t) = i[\mathcal{H}(0), S^\pm_n] \mp h \ S^z_n, \quad \frac{d}{dt} S^z_n(t) = i[\mathcal{H}(0), S^z_n]. \quad (A.2)$$

Equations (A.2) permit us to express the dynamical susceptibilities for $h \neq 0$ in terms of the ones in zero field

$$\chi^{+,-}(\omega, q, h) = \chi^{+,-}(\omega - h, q, 0),$$
$$\chi^{-,+}(\omega, q, h) = \chi^{-,+}(\omega + h, q, 0),$$
$$\chi^{zz}(\omega, q, h) = \chi^{zz}(\omega, q, 0). \quad (A.3)$$

This implies that the structure factors in a field are simply the same as those in zero field apart from constant shifts in energy. The leading contributions to the dynamical susceptibilities in zero field have been calculated in the framework of the $O(3)$ nonlinear-sigma model approximation to the isotropic spin-1 Heisenberg chain in [23, 41]. It follows from these results that the three-particle contributions are very small. We note that the threshold of the $M_+ M_+ M_-$ three-particle continuum (two $S^z = 1$ magnons and one $S^z = -1$ magnon) is at $3\Delta - h$, i.e. for any $H < H_c$ it still is very slightly higher in energy than the highest energy $M_-$ magnon mode. Hence all three magnon modes remain ‘sharp’ for all $H < H_c$.

We note that analogous considerations apply in the presence of a single-ion anisotropy in the $z$-direction only ($E = 0$ in (1.1) and a magnetic field along the $z$-direction). The dynamical susceptibilities for finite fields can then be expressed in terms of the zero field susceptibilities through the equation of motions for the spin operators. This is quite useful for the Majorana fermion model, where the staggered components of the spin operators are
Haldane-gap chains in a magnetic field

expressed in terms of Ising order and disorder operators. The latter transform nontrivially under the Bogoliubov transformation used to diagonalize the Hamiltonian for nonzero magnetic fields.

Appendix B: Spectral representation of correlation functions

In this appendix we collect useful formulae for spectral representations of correlation functions in massive, integrable, relativistic quantum field theories.

We parametrize energy and momentum of single particle states in terms of a rapidity variable

\[ E_\epsilon(\theta) = \Delta_\epsilon \cosh \theta, \quad P_\epsilon(\theta) = \frac{\Delta_\epsilon}{v} \sinh \theta. \]

(B.1)

Here the index \( \epsilon \) labels the different types of particles and \( \Delta_\epsilon \) are the corresponding spectral gaps. A scattering state of \( N \) particles with rapidities \( \{\theta_j\} \) and indices \( \{\epsilon_j\} \) is denoted by

\[ |\theta_1, \theta_2, \ldots, \theta_N\rangle_{\epsilon_1, \epsilon_2, \ldots, \epsilon_N}. \]

(B.2)

Its energy and momentum are

\[ E(\{\theta_j\}) = \sum_{j=1}^{N} \Delta_{\epsilon_j} \cosh \theta_j, \quad P(\{\theta_j\}) = \frac{\sum_{j=1}^{N} \Delta_{\epsilon_j}}{v} \sinh \theta_j. \]

(B.3)

A basis of states is most easily constructed in terms of the generators of the so-called Faddeev–Zamolodchikov algebra

\[
Z^\dagger_{\epsilon_1}(\theta_1)Z_{\epsilon_2}(\theta_2) = S^\epsilon_{\epsilon_1, \epsilon_2}(\theta_1 - \theta_2)Z^\epsilon_{\epsilon_2}(\theta_2)Z^\epsilon_{\epsilon_1}(\theta_1),
\]

\[
Z^\dagger_{\epsilon_1}(\theta_1)Z^\dagger_{\epsilon_2}(\theta_2) = \frac{1}{\sqrt{2}i}S^\epsilon_{\epsilon_1, \epsilon_2}(\theta_2 - \theta_1)Z^\epsilon_{\epsilon_2}(\theta_2)Z^\epsilon_{\epsilon_1}(\theta_1) + 2\pi \delta^\epsilon_{\epsilon_1, \epsilon_2}(\theta_1 - \theta_2).
\]

(B.4)

Here \( S^\epsilon_{\epsilon_1, \epsilon_2}(\theta) \) is the factorizable two-particle scattering matrix of the integrable quantum field theory. Using theZF operators a Fock space of states can be constructed as follows. The vacuum is defined by

\[ Z_{\epsilon_i}(\theta)|0\rangle = 0. \]

(B.5)

Multiparticle states are then obtained by acting with strings of creation operators \( Z^\dagger_{\epsilon_i}(\theta) \) on the vacuum

\[ |\theta_n, \ldots, \theta_1\rangle_{\epsilon_n, \ldots, \epsilon_1} = Z^\dagger_{\epsilon_n}(\theta_n) \cdots Z^\dagger_{\epsilon_1}(\theta_1)|0\rangle. \]

(B.6)

The resolution of the identity in the normalization implied by (B.4) is given by

\[
1 = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\{\epsilon_j\}} \int_{-\infty}^{\infty} \prod_{j=1}^{n} \frac{d\theta_j}{2\pi} |\theta_n, \ldots, \theta_1\rangle_{\epsilon_n, \ldots, \epsilon_1} \langle \theta_1, \ldots, \theta_n|. \]

(B.7)
The two point function of some operator $\mathcal{O}$ can now be expressed in the spectral representation as

$$
\langle \mathcal{O}(t,x)\mathcal{O}(0,0) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\epsilon_j} \int_{-\infty}^{\infty} \prod_{j=1}^{n} \frac{d\theta_j}{2\pi} |f_{\epsilon_1,\ldots,\epsilon_n}(\theta_1,\ldots,\theta_n)|^2 \times \exp(-itE(\{\theta_j\})) + i\epsilon(\{\theta_j\}),
$$

where the form factors are given by

$$
f_{\epsilon_1,\ldots,\epsilon_n}(\theta_1,\ldots,\theta_n) \equiv \langle 0|\mathcal{O}^\dagger(0,0)|\theta_n,\ldots,\theta_1\rangle_{\epsilon_n,\ldots,\epsilon_1}.
$$

**Appendix C: Bound states in the Majorana model**

In this appendix we address the question of whether the current–current interaction in the Majorana model leads to the formation of bound states. For simplicity we consider only the $SU(2)$ symmetric case with Hamiltonian

$$
\mathcal{H} = \frac{i}{2} \int dt \sum_{a=1}^{3} v[L_a \partial_t L_a - R_a \partial_t R_a] - 2mR_aL_a + g \int dt \sum_a J^a J^a.
$$

We aim to establish that bound states exist for any $g > 0$, whereas there are no bound states for $g < 0$. We recall that the Majorana fermion model arises from the spin-Heisenberg Hamiltonian with an additional biquadratic term

$$
\mathcal{H}_{\text{biquad}} = J \sum_n S_n \cdot S_{n+1} - b(S_n \cdot S_{n+1})^2,
$$

where $|b - 1| \ll 1$. For $b > 1$ the model is in a dimerized phase whereas $b < 1$ corresponds to a Haldane spin-liquid regime. One may establish by using the expressions (2.5) for the spin operators that the case $b < 1$ ($b > 1$) corresponds to $g < 0$ ($g > 0$). In order to determine whether the current–current interaction leads to the formation of bound states, we first consider the limit of a very anisotropic interaction

$$
\mathcal{H}_{\text{ani}} = \frac{i}{2} \int dt \sum_{a=1}^{3} v[L_a \partial_t L_a - R_a \partial_t R_a] - 2mR_aL_a + g \int dt \sqrt{J^a J^a}.
$$

This case can be mapped onto a single massive Majorana fermion plus the massive Thirring model by introducing complex Fermi fields by

$$
R_1 = \frac{\Psi_R + \Psi_R^\dagger}{\sqrt{2}}, \quad R_2 = \frac{\Psi_R - \Psi_R^\dagger}{i\sqrt{2}},
$$

$$
L_1 = \frac{\Psi_L - \Psi_L^\dagger}{i\sqrt{2}}, \quad L_2 = \frac{\Psi_L + \Psi_L^\dagger}{\sqrt{2}}.
$$

The Hamiltonian density is rewritten as $\mathcal{H}_{\text{ani}} = \mathcal{H}_{\text{Maj}} + \mathcal{H}_{\text{MTM}}$, where

$$
\mathcal{H}_{\text{Maj}} = \frac{iv}{2} \int dt \left[ L_3 \partial_t L_3 - R_3 \partial_t R_3 - \frac{2m}{v} R_3 L_3 \right],
$$

$$
\mathcal{H}_{\text{MTM}} = -iv \int dt \left[ \Psi_R^\dagger \partial_t \Psi_R - \Psi_L^\dagger \partial_t \Psi_L \right] + \int dt \left[ m[\Psi_R^\dagger \Psi_L + \text{h.c.}] + 2g \Psi_L^\dagger \Psi_L \Psi_R^\dagger \Psi_R \right].
$$
In equation (C.5) we have dropped a term proportional to \( \int dx [\Psi_R^\dagger \Psi_R + \Psi_L^\dagger \Psi_L] \) as it commutes with the Hamiltonian. It is well known that in the massive Thirring model there are breather bound states for \( g > 0 \), but no bound states exist for \( g < 0 \), see e.g. [43].

A different approach is to use large-\( N \) methods. If we consider \( N \) species of Majorana fermions rather than three, we may decouple the interaction through a bosonic Hubbard–Stratonovich field \( \sigma \). For even \( N \) and \( g > 0 \) the problem maps onto the \( O(N/2) \) massive Gross–Neveu model, which is known to have bosonic bound states in the large-\( N \) limit [44].

**Appendix D: Low-energy projections of the staggered magnetizations**

In this appendix we give arguments in favour of the identification (4.6) at low energies and in the vicinity of the Ising critical point at \( H = H_c \). We first consider the LG theory and then the Majorana fermion model.

**D.1. Landau–Ginzburg model**

It is instructive to examine the evolution of the amplitudes \( A_{aa} \) entering the mode expansions (3.7) of the scalar fields \( \varphi_a \) as the magnetic field is increased. We recall that the critical field is \( H_c = \Delta_1 \). In the vicinity of \( H_c \) we parametrize

\[
H = \Delta_1 - \delta, \quad \delta > 0.
\]

As we are interested only in low energies we may restrict our attention to the ‘−’ modes. From (3.10) we obtain the following expansions in \( \delta \)

\[
(\omega_-(0))^2 \approx \frac{2\Delta_1(\Delta_2^2 - \Delta_1^2)}{3\Delta_1^2 + \Delta_2^2} \delta,
\]

\[
\left[ \frac{A_{2-}(0)}{A_{1-}(0)} \right]^2 = \frac{(7\Delta_1^2 + 3\Delta_2^2)\delta}{2\Delta_1(3\Delta_1^2 + \Delta_2^2)}.
\]

Equations (D.2) imply that close to \( H_c \) we have

\[
A_{2-}(0) \propto \omega_-(0) A_{1-}(0).
\]  

(D.3)

As we have seen before, close to \( H_c \) the \( x \)-component of the staggered magnetization \( \varphi_1 \) couples to \( M_- \) with a finite amplitude \( A_{1-}(0) \) given by (3.11). Furthermore we have the identification (4.6)

\[
\varphi_1 \propto \sigma,
\]  

(D.4)

where \( \sigma \) is the Ising order parameter field. Equations (D.3) and (D.4) together suggest that

\[
\varphi_2 \propto \partial_t \sigma.
\]  

(D.5)

This claim may be substantiated further in the limit where one of the zero field gaps is much smaller than the other, i.e. \( \Delta_1 \ll \Delta_2 \). As we are interested in energies that are small compared to \( \Delta_2 \), we may ‘integrate out’ the high-energy degrees of freedom corresponding to \( \varphi_2 \) in the path integral expression for the staggered magnetization \( n^y \). Because \( H_c = \Delta_1 \)
is small, we may furthermore take the magnetic field into account perturbatively. The staggered magnetization in the $y$-direction is

$$n^y(t, x) = \varphi_2(t, x).$$

(A.6)

Averaging $n^y(t, x)$ over $\varphi_2$, we obtain

$$\langle n^y(t, x) \rangle_2 = \frac{1}{Z} \int D\varphi_2 \varphi_2(t, x) \exp\left[ \frac{S_2 - 2i(H/v) \int dt_1 dx_1 [\varphi_2 \partial_{t_1} \varphi_1]}{2} \right],$$

where

$$S_2 = \int dt dx \left[ \frac{1}{2v} (\partial_t \varphi_2)^2 - \frac{v}{2} (\partial_x \varphi_2)^2 - \frac{\Delta_2^2}{2v} \varphi_2^2 \right].$$

(D.8)

The leading contribution occurs in first order in the magnetic field

$$\langle n^y(t, x) \rangle_2 \approx -\frac{2iH}{v} \int dx_1 dt_1 \langle T \varphi_2(t, x) \varphi_2(t_1, x_1) \rangle_2 \partial_t \varphi_1(t_1, x_1)$$

$$= \frac{2H}{v} \int dx_1 dt_1 G_2(t - t_1, x - x_1) \partial_t \varphi_1(t_1, x_1)$$

$$\approx \frac{2H}{v} \left[ \int dx' \int dt'_1 G_2(t'_1, x'_1) \right] \partial_t \varphi_1(t, x).$$

(D.9)

In the last line we have used that the leading contribution to the integral comes from the region $t_1 \approx t, x_1 \approx x$. This shows that the mixing induced by the magnetic field generates a contribution to $n^y(t, x)$ proportional to $\partial_t \varphi_1(t, x)$ at low energies.

**D.2. Majorana fermion model**

Analogous calculations can be performed in the framework of the Majorana fermion model in the case $g_a = 0$, i.e. in the absence of the current–current interactions. In particular, let us consider the case where one of the zero field gaps is much smaller than the other

$$\Delta_1 \ll \Delta_2.$$

(D.10)

As the critical field $H_c = \sqrt{\Delta_1 \Delta_2}$ is much smaller than $\Delta_2$ we may treat the magnetic field term perturbatively. We may derive an effective action for $R_1, L_1$ only by integrating out $R_2$ and $L_2$ (we recall that the third Majorana decouples in the absence of interactions)

$$S_{\text{eff}} \approx S_1 - \frac{1}{2} \langle S_{H}^2 \rangle_2,$$

$$S_H = iH \int dx d\tau \left[ L_1 L_2 + R_1 R_2 \right],$$

where $\langle \rangle_2$ denotes the expectation value with respect to the second Majorana fermion and

$$S_1 = \int d\tau dx \left[ R_1 \partial_- R_1 + L_1 \partial_+ L_1 - i\Delta_1 R_1 L_1 \right],$$

$$\partial_\pm = \frac{\partial_x \pm iv \partial_t}{2}.$$
The Matsubara Green functions are defined as e.g.
\[ G_{RR}(\tau, x) = -(T, R(\tau, x)R(0)). \] (D.13)

Their Fourier transforms are
\[ G_{R_1R_2}(\omega, q) = -\frac{i\omega + vq}{\omega^2 + v^2q^2 + \Delta^2}, \]
\[ G_{L_1L_2}(\omega, q) = -\frac{i\omega - vq}{\omega^2 + v^2q^2 + \Delta^2}, \] (D.14)
\[ G_{R_3L_2}(\omega, q) = +\frac{i\Delta_2}{\omega^2 + v^2q^2 + \Delta^2}. \]

A straightforward calculation then gives
\[ \mathcal{L}_{\text{eff}} = R_1 \partial_- R_1 + L_1 \partial_+ L_1 - i \left[ \Delta_1 - \frac{H^2}{\Delta_2} \right] R_1 L_1. \] (D.15)

In other words, integrating out the second Majorana leads to a renormalization of the mass of the first Majorana. We note that the dispersion relation that follows from (D.15) agrees with the expansion of \( \omega_+(q) \) (2.20) in the case \( H \ll \Delta_2 \) as it must. What we have shown is that in the case \( \Delta_1 \ll \Delta_2 \) it is simply the first Majorana that becomes critical at \( H_c \). The staggered magnetization in the \( x \)-direction is expressed at low energies by averaging (2.6) with respect to the second and third Majoranas, which gives
\[ n^x(x) \propto \sigma^1(x) \langle \mu^3(x) \rangle \langle \mu^3(x) \rangle. \] (D.16)

The determination of the operator content of \( n^y(x) \) at low energies is significantly more involved. In order to obtain the low-energy projection, we need to average with respect to the second and third Majoranas
\[ n^y(0, 0) \approx -iH \langle \mu_3 \rangle \int d\tau dx \left\{ \langle L_2(\tau, x)\sigma_2(0) \rangle L_1(\tau, x)\mu_1(0) \right. \]
\[ + \left. \langle R_2(\tau, x)\sigma_2(0) \rangle R_1(\tau, x)\mu_1(0) \right\}. \] (D.17)

The expectation values \( \langle \_ \rangle_2 \) with respect to the second Majorana can be evaluated by the form factor bootstrap approach by utilizing the results of [20]–[22]. We obtain
\[ \langle L_2(\tau, x)\sigma_2(0) \rangle_2 \approx D e^{i\pi/4} \frac{1}{\sqrt{v\tau + i\epsilon}} e^{-m\tau}, \]
\[ \langle R_2(\tau, x)\sigma_2(0) \rangle_2 \approx D e^{-i\pi/4} \frac{1}{\sqrt{v\tau - i\epsilon}} e^{-m\tau}, \] (D.18)

where \( D = m^{1/8}(4\pi)^{-1/2}2^{1/12}e^{-1/8}A^{3/2} \) and \( r^2 = \tau^2 + x^2/v^2 \). Using these results in (D.17) we see that the integral is dominated with exponential accuracy by the region \( \tau \approx 0, x \approx 0 \). Hence the operator content of \( n^y \) is determined by the fusion of the disorder operator \( \mu_1 \) with the left and right moving fermions \( L_1, R_1 \). The relevant operator product expansions can be worked out following [45]
\[ L(\tau, x)\mu(0) \approx \frac{\gamma}{\sqrt{\epsilon}} \sigma(0) - \frac{m\gamma}{v} \sqrt{\epsilon} \sigma(0) + \frac{4\gamma}{v} \sqrt{\epsilon} \partial_- \sigma(0), \]
\[ R(\tau, x)\mu(0) \approx \frac{\gamma}{\sqrt{\epsilon}} \sigma(0) - \frac{m\gamma}{v} \sqrt{\epsilon} \sigma(0) + \frac{4\gamma}{v} \sqrt{\epsilon} \partial_+ \sigma(0). \] (D.19)
Haldane-gap chains in a magnetic field

where \( z = v \tau + ix, \gamma = \exp(-i\pi/4)/\sqrt{4\pi} \) and \( \partial_\pm = \frac{1}{2}(\partial_\tau \mp iv\partial_x). \) Combining (D.18) with (D.19) we obtain the desired result

\[
n^y \propto \partial_\tau \sigma.
\]  
(D.20)

Appendix E: Derivation of the sine-Gordon model in the high-field phase for weak anisotropy

In this appendix we show how the sine-Gordon Hamiltonian emerges as the low-energy effective theory at \( H > H_c \) in the small anisotropy limit \( \Delta_2 - \Delta_1 \ll H - H_c. \) We first present a derivation in the framework of the nonlinear sigma model and then within the Majorana fermion model.

E.1. Nonlinear sigma model

The isotropic spin-\( S \) Heisenberg chain in a magnetic field can be mapped onto the \( O(3) \) nonlinear sigma model in the continuum limit. Exploiting the integrability of the nonlinear sigma model it was shown in \([13]\) that for \( H > \Delta \) the low-energy regime is described in terms of a free boson

\[
\mathcal{H} = \frac{\tilde{v}}{16\pi} \int dx \left[ (\partial_x \Phi)^2 + (\partial_x \Theta)^2 \right].
\]  
(E.1)

Here \( \Theta \) is the field dual to \( \Phi \) and fulfils

\[
\tilde{v}\partial_x \Theta = -i\partial_\tau \Phi, \quad \partial_\tau \Theta = i\tilde{v}\partial_x \Phi.
\]  
(E.2)

The low-energy behaviour of spin correlations follows from the correspondence

\[
S_n^\pm \simeq (-1)^n A \exp \left( \pm i\frac{\beta}{2} \Theta \right).
\]  
(E.3)

The parameters \( \tilde{v} \) and \( \beta \) were calculated in \([13]\). Adding a very small crystal field anisotropy to the Hamiltonian

\[
E \sum_j [(S_j^x)^2 - (S_j^y)^2]
\]  
(E.4)

generates a term proportional to

\[
\int dx \cos(\beta \Theta).
\]  
(E.5)

The resulting theory is the sine-Gordon model (5.3). The term \( D \sum_j (S_j^z)^2 \) merely leads to a small change in \( \beta \) which we ignore here.
E.2. Majorana fermion model

Our starting point is the Hamiltonian (2.14) describing the two Majorana fermions that couple to the magnetic field in the limit $\Delta_2 = \Delta_1 = m$, i.e. vanishing gap anisotropy $\Delta = 0$. Using

$$\Psi_{R,L} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} c_{R,L}(k),$$

(E.6)

we may express the Hamiltonian as

$$H_{12}|_{\Delta=0} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} (c^\dagger_R, c^\dagger_L) M \begin{pmatrix} c_R \\ c_L \end{pmatrix} ,$$

(E.7)

where

$$M = \begin{pmatrix} vk + H & -im \\ im & -vk + H \end{pmatrix} .$$

(E.8)

Now we may carry out a Bogoliubov transformation

$$\begin{pmatrix} a_k \\ b_k \end{pmatrix} = \begin{pmatrix} \cos(\varphi_k) & -i \sin(\varphi_k) \\ -i \sin(\varphi_k) & \cos(\varphi_k) \end{pmatrix} \begin{pmatrix} c_R(k) \\ c_L(k) \end{pmatrix} ,$$

(E.9)

with

$$\tan(2\varphi_k) = \frac{m}{vk}$$

(E.10)

to diagonalize the Hamiltonian. We find

$$H_{12}|_{\Delta=0} = \int \frac{dk}{2\pi} \left[ \left( H + \text{sgn}(k)\sqrt{m^2+v^2k^2} \right) a^\dagger_k a_k + \left( H - \text{sgn}(k)\sqrt{m^2+v^2k^2} \right) b^\dagger_k b_k \right] .$$

(E.11)

Introducing fermions $c$ and $d$ by

$$c(k) = a_k \theta(k) + b_k \theta(-k), \quad d(k) = b_k \theta(k) + a_k \theta(-k),$$

(E.12)

we may express the Hamiltonian (E.11) as

$$H_{12}|_{\Delta=0} = \int \frac{dk}{2\pi} \left[ \left( H + \sqrt{m^2+v^2k^2} \right) c^\dagger(k)c(k) + \left( H - \sqrt{m^2+v^2k^2} \right) d^\dagger(k)d(k) \right] .$$

(E.13)

The low-energy modes occur in the lower band in the vicinity of $\pm k_F = \pm \sqrt{(H^2-m^2)/v^2}$. They can be combined into left and right moving Fermi fields by

$$d(x) = \exp(-ik_Fx)R(x) + \exp(ik_Fx)L(x).$$

(E.14)

The low-energy effective Hamiltonian is then

$$\mathcal{H}' = i\bar{w} \int dx \left[ L^\dagger \partial_x L - R^\dagger \partial_x R \right] ,$$

(E.15)
where $\tilde{v} = v^2 k_F / H$. We now bosonize the low-energy Hamiltonian using

$$
R^\dagger(x) \sim \frac{1}{\sqrt{2\pi}} \exp\left(\frac{i \Phi(x) + \Theta(x)}{2\sqrt{2}}\right),
$$

$$
L^\dagger(x) \sim \frac{1}{\sqrt{2\pi}} \exp\left(-i \frac{\Phi(x) - \Theta(x)}{2\sqrt{2}}\right). \tag{E.16}
$$

We find

$$
\mathcal{H}' = \frac{\tilde{v}}{10\pi} \int dx \left[ (\partial_x \Phi)^2 + (\partial_x \Theta)^2 \right]. \tag{E.17}
$$

The high-energy cutoff in this construction is given by the depth of the Fermi sea in the lower band of (E.11), which is $H - \mu = H - H_c$. So far we have neglected the gap anisotropy, i.e. the term

$$
\mathcal{H}_{\text{pair}} = i \Delta \int dx \left[ \Psi_R^\dagger \Psi_L^\dagger - \text{h.c.} \right]. \tag{E.18}
$$

in the Hamiltonian (2.14). In the next step we take it into account under the assumption that $\Delta$ is small compared to the cutoff $H - H_c$. In this limit $\mathcal{H}_{\text{pair}}$ is expressed in terms of the modes as

$$
\mathcal{H}_{\text{pair}} = i \Delta \int_0^\infty \frac{dk}{2\pi} \left[ c_R^\dagger(k) c_L^\dagger(-k) - c_L(-k) c_R(k) \right]. \tag{E.19}
$$

After the Bogoliubov transformation this becomes

$$
- i \Delta \int_0^\infty \frac{dk}{2\pi} \cos(2\varphi_k) \left[ d(k)d(-k) - c(k)c(-k) - \text{h.c.} \right] + \text{mixed terms}. \tag{E.20}
$$

Dropping the ‘high-energy’ filled band as well as the mixed terms (they contribute in higher orders of $\Delta/(H - H_c)$) we have

$$
\mathcal{H}'_{\text{pair}} \simeq - i \Delta \int_0^\infty \frac{dk}{2\pi} \frac{vk}{\sqrt{m^2 + v^2 k^2}} \left[ d(k)d(-k) - \text{h.c.} \right]. \tag{E.21}
$$

Expanding around $\pm k_F$ this can be rewritten in terms of the left and right moving fermions as

$$
\mathcal{H}'_{\text{pair}} \simeq i \Delta \sqrt{1 - \frac{m^2}{H^2}} \int dx \left[ RL - L^\dagger R^\dagger \right]. \tag{E.22}
$$

Finally, bosonization gives

$$
\mathcal{H}'_{\text{pair}} \simeq - \frac{\Delta}{\pi} \sqrt{1 - \frac{m^2}{H^2}} \int dx \cos\left(\frac{\Theta}{\sqrt{2}}\right). \tag{E.23}
$$

By combining equations (E.17) and (E.23) we see that in the absence of interactions the Majorana fermion model gives rise to a sine-Gordon effective theory at low energies in the parameter regime we have been discussing. The parameter $\beta$ in (5.3) takes the special free-fermionic value $\beta = 1/\sqrt{2}$.

Interactions can be treated in a way analogous to the pairing term. If we drop the interaction terms involving the third Majorana (which we assume to have the largest gap)
the interaction Hamiltonian reads
\[ H_{\text{int}} = -2g_3 \int dx \, L_1 L_2 R_1 R_2, \quad (E.24) \]
where \( g_3 < 0 \). Expressing this in terms of the complex fields \( \Psi_{R,L} \), carrying out a mode expansion and subsequent Bogoliubov transformation and finally projecting to the low-energy band we obtain
\[ H'_{\text{int}} \simeq 2g_3 \frac{v^2 k_F^2}{m^2 + v^2 k_F^2} \int dx \, R^\dagger RL, \quad (E.25) \]
where \( R \) and \( L \) have been introduced in (E.14). Bosonization then gives
\[ H'_{\text{int}} \simeq \frac{g'_3 \tilde{v}}{16\pi} \int dx \, \left[ (\partial_x \Phi)^2 - (\partial_x \Theta)^2 \right], \quad (E.26) \]
where \( g'_3 = g_3 \tilde{v}/\pi v^2 \). This term may be combined with (E.17) by rescaling the scalar fields in the standard way
\[ \Phi \rightarrow \left[ 1 - g'_3 \right]^{1/4} \Phi, \quad \Theta \rightarrow \left[ 1 + g'_3 \right]^{1/4} \Theta. \quad (E.27) \]
In terms of the rescaled fields the total Hamiltonian takes the form of a sine-Gordon model (5.3) (with a slightly changed velocity) where
\[ \beta = \frac{1 + g'_3 - g'_3}{1 - g'_3} \quad \frac{1}{\sqrt{2}} < \frac{1}{\sqrt{2}}. \quad (E.28) \]
Hence the sine-Gordon model is in the attractive regime.

**Appendix F: Correlation amplitude in the commensurate–incommensurate transition**

Let us consider the LG model (3.1) in the \( U(1) \) symmetric case \( \Delta_1 = \Delta_2 = \Delta_3 = m \). For \( H > H_c = m \) the low-energy degrees of freedom are described by a Luttinger liquid, which can be derived by means of Haldane’s harmonic fluid approach [25] as follows. Forming a complex Bose field out of the two components of the LG field that couple to the magnetic field
\[ \Psi_B = \frac{\varphi_1 + i\varphi_2}{\sqrt{2}}, \quad (F.1) \]
and then bosonizing using [25]
\[ \Psi_B^\dagger \simeq \sqrt{\rho_0 + a_0} \Pi \left[ \sum_{m \text{ even}} e^{i m \Phi} \right] e^{i\Theta} \quad (F.2) \]
one obtains, after rescaling the fields \( \Phi \) and \( \Theta \), a Lagrangian density of the form [14]
\[ \mathcal{L} = \frac{1}{16\pi} \left[ \frac{1}{\tilde{v}} \left( \frac{\partial \Theta}{\partial t} \right)^2 - \tilde{v} \left( \frac{\partial \Theta}{\partial x} \right)^2 \right]. \quad (F.3) \]
Here $\tilde{v} = 2v\sqrt{2((H - m)/m)}$, $\rho_0$ is the (dimensionless) boson density, which corresponds to the magnetization per site and $\Pi$ is the momentum conjugate to $\Theta$. As the LG fields $\varphi_a$ are the staggered components of the spin operators we conclude that

$$S_j^\pm \propto (-1)^j A \exp\left(\pm \frac{i\beta \Theta}{2}\right), \quad (F.4)$$

where $\beta$ depends on the magnetization and is related to the parameter $\eta$ of [14] by $\beta^2 = \eta$. By virtue of (F.2) the amplitude $A$ is proportional to

$$A \propto \sqrt{\rho_0 a \beta^2}, \quad (F.5)$$

where $a$ is a short-distance cutoff and vertex operators are normalized according to (5.6). The short-distance cutoff is

$$a = a_0 \rho_0 \quad (F.6)$$

We note that the short-distance cutoff (F.6) diverges as $H$ approaches $m$ as $\rho_0 \to 0$ and (F.4) describes the asymptotic behaviour of spin correlation functions at distances much larger than $a$. Combining (F.6) and (F.5) we find that in general we have [25]

$$A \propto \rho_0^{(1-\beta^2)/2}. \quad (F.7)$$

Let us now specialize to magnetic fields very close to the critical field $H_c = m$

$$H - m \ll m. \quad (F.8)$$

As shown in [25], the parameter $\beta$ tends to $1/\sqrt{2}$, so that

$$S_j^\pm \propto (-1)^j A \exp\left(\pm \frac{i\Theta}{2\sqrt{2}}\right), \quad (F.9)$$

where the density is given by [14]

$$\rho_0 = \frac{a_0}{\pi v} \sqrt{2m(H - m)}. \quad (F.10)$$

Combining (F.10), (F.6) and (F.5) we obtain

$$A = A' a_0^{1/4} \left[\frac{H - H_c}{J}\right]^{1/8}, \quad (F.11)$$

where $A'$ is a numerical, field independent constant and where we have used that $v^2/ma_0^2 \propto J$. The field dependence of the correlation amplitude (F.11) is a universal feature of the C–IC transition.

Let us apply these ideas to another example of the C–IC transition: the spin-1/2 Heisenberg XXZ chain in a longitudinal magnetic field

$$\mathcal{H}_{XXZ} = J \sum_n S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \delta S_n^z S_{n+1}^z + H \sum_n S_n^z, \quad (F.12)$$

where $-1 < \delta \leq 1$. The model (F.12) has a phase transition from a gapless, in-commensurate Luttinger liquid phase to a gapped, commensurate, spin-polarized phase.
at a critical value

\[ H_c = J(1 + \delta). \]  

(F.13)

Slightly below this transition, i.e.

\[ 0 < 1 - \frac{H}{H_c} \ll 1, \]

(F.14)

the transverse correlation functions exhibit the following large-distance asymptotics

\[ \langle S^x_1(0)S^x_{R+1}(0) \rangle \sim (-1)^R \frac{e^{1/2}2^{11/12} \left([H_c - H]/J\right)^{1/4}}{R^{1/2}}, \]  

(F.15)

where \( A \) is Glaisher’s constant (4.12). This result is obtained as follows: the dependence on the magnetic field is universal and given by (F.11). The numerical coefficient is fixed by noting that the numerical results of [18] show that \( A' \) is independent of the value of the anisotropy \( \delta \). Finally, we use that the correlation amplitude has been calculated for the free fermion case in [46]. The result (F.15) is in good agreement with the numerical results of [18] in the close proximity of the transition, as was already noted in [18].

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