Field-Induced Ising Criticality and Incommensurability in Anisotropic Spin-1 Chains

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Quantum phase transitions induced by an external magnetic field in the Haldane-gapped spin-1 chains are studied in a fermionic field-theoretic description of the model. In the case with broken axial symmetry, two transitions occur consecutively as increasing the field: $h_c = (m_1 m_2)_{1/2}$ (with $m_1$ and $m_2$ the transverse masses) is the critical Ising point and $h'_c > h_c$ is the commensurate-incommensurate transition point. Although the latter is thermodynamically indiscernible, its property is revealed in the spin correlation functions (both uniform and staggered) which are calculated upon expressing the correlations of coupled Ising pair fields in terms of block-Toeplitz determinants.

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It is now well established that a one-dimensional (1D) quantum antiferromagnet with spin-1 possesses a (Haldane) gap in the excitation spectrum which separates the first excited triplet states from the singlet ground state [1]. The elementary excitations are coherent antiferromagnetic massive magnons appearing around $q = \pi$ and carrying quantum number $S = 1$. If an external magnetic field is introduced into the Haldane system, the transverse modes couple to the field and phase transition may occur when the field overcomes the gap [2-4]. Experimentally, there have indeed been observed phase transitions in some quasi-1D compounds by measuring specific heat [9, 10], as well as neutron scattering [7, 11, 12].

For an isotropic chain or the field applied having axial symmetry, a commensurate-incommensurate (C-IC) transition [13] takes place when the field surpasses the gap. Aside from magnetization, the external field induces a planar quasi-long-range order in the staggered spin correlations. The correlation peak [7, 11, 12], as well as neutron scattering [10], associated with the commensurate-incommensurate transition point. Although the latter is thermodynamically indiscernible, its property is revealed in the spin correlation functions (both uniform and staggered) which are calculated upon expressing the correlations of coupled Ising pair fields in terms of block-Toeplitz determinants. The magnetic field coupling to the uniform spin density contributes a Zeeman energy as $H_{\text{Ising}}(x) = h I^z(x) = -i\hbar(\xi^1_R \xi^2_R + \xi^1_L \xi^2_L)$, which apparently only mixes first two (transverse) species of Majoranas, and the third one drops out of the system as a free massive Majorana, or equivalently, off-critical Ising model. Therefore, we need only concentrate on the Hamiltonian

$$H(x) = \sum_{\alpha=1,2} \left[ -\frac{i\hbar}{2}(\xi^\alpha_R \partial_x \xi^\alpha_L - \xi^\alpha_L \partial_x \xi^\alpha_R) - im_\alpha \xi^\alpha_R \xi^\alpha_L \right] - i\hbar(\xi^1_R \xi^2_R + \xi^1_L \xi^2_L).$$

(1)

Denoting $m = \frac{1}{2}(m_1 + m_2)$ and $\Delta = \frac{1}{2}(m_1 - m_2)$ and combining two Majoranas into a Dirac fermion, model (1) actually describes a charge density wave-Cooper pairing-chemical potential ($m-\Delta-h$) system in 1D. When bosonized, it becomes a sine-Gordon model with extra terms of dual field and field derivative.

While the uniform spin correlations are easy to compute, it is not the case for the staggered part, since they are composed of Ising order and disorder fields, which are...
related to the Majorana fermions in a highly non-trivial way (Jordan-Wigner transformation). To exploit the full advantage of the solvableness of the model, we regularize on a 1D lattice, on which the relations between the Ising variables and the fermions can be unambiguously established. By using the relations between the Majorana fields and the lattice Dirac fermion:

\[
\begin{align*}
\xi_R &\rightarrow -\frac{1}{\sqrt{2a}}(e^{i\pi/4}c_n + e^{-i\pi/4}c_n), \\
\xi_L &\rightarrow \frac{1}{\sqrt{2a}}(e^{-i\pi/4}c_n + e^{i\pi/4}c_n),
\end{align*}
\]

(2)

we have the following lattice version of two coupled quantum Ising chains (QICs) (or \(m\)-\(\Delta\)-\(h\) model):

\[
H = H_{\text{QIC}}^{[a]} + H_{\text{QIC}}^{[b]} - ih \sum_n (a_n^\dagger b_n - b_n^\dagger a_n),
\]

(3)

where \(H_{\text{QIC}}^{[a]} = \frac{J}{2} \sum_n [(c_n^\dagger - c_n)(c_{n+1}^\dagger + c_{n+1}) - \lambda_c (c_n^\dagger - c_n)(c_n^\dagger + c_n)]\) with parameters \(J = \frac{w}{a}\) and \(\lambda_c = 1 + \frac{m}{r}\) (\(c = (1, 2) = (a, b)\)). Without loss of generality, we assume \(m_1 \geq m_2 > 0\) (so that \(m > \Delta \geq 0\) and \(\lambda > 1\)) and \(h \geq 0\) unless otherwise stated. The units are so chosen that \(J = 1\).

Model \(\mathfrak{K}\) is diagonalized through a unitary transformation and the spectrum is found to be

\[
E_k^2 = (\Theta_k^2 \pm \Gamma_k^2)^{1/2},
\]

(4)

where \(\Theta_k^2 = \Delta^2 + h^2\) and \(\Gamma_k^2 = (\Delta^2 + h^2)^{1/2}\) with \(\Delta^2 = \epsilon_k^2 + \sin^2 k\) and \(\epsilon_k = \cos k - \lambda\). There exist totally six (real) correlation functions for the fermions:

\[
\begin{align*}
C_1^a(n) &= \langle c_n^\dagger c_0 \rangle, & C_2^a(n) &= \langle c_n^\dagger c_{n+1}^\dagger \rangle, & (c = a, b) \\
C_3(n) &= \langle i(a_n^\dagger b_n) \rangle, & C_4(n) &= -i(a_n b_n).
\end{align*}
\]

(5)

The explicit forms of these correlations are obtained in a variational approach, and all of them are 1D integrations over momentum. To calculate the correlations of the coupled Ising fields, we need further

\[
\begin{align*}
G_{a,b}^n &= -\delta_{ab} + 2[C_{a,b}^1(n) - C_{a,b}^2(n)], \quad \text{(real)} \\
F_n &= 2i[C_3(n) - C_4(n)]. \quad \text{(imaginary)}
\end{align*}
\]

(6)

As is well-known, the correlation functions of the QIC can be expressed as the so-called Toeplitz determinants. A Toeplitz matrix has its elements parallel to the diagonal the same value, i.e., it takes the form \(\mathcal{T} = [f_T(i-j)]\). We find that for the two QICs coupled in the present fashion, the correlation of a pair of Ising fields can be cast into a block-Toeplitz form with a doubled size. To this purpose, we introduce following seven \(r \times r\) Toeplitz matrices:

\[
\begin{align*}
\hat{G}_{\sigma}^{a,b}(r) &= [-G_{i-j+1}^{a,b}], & \hat{F}_{\sigma}(r) &= [-F_{i-j+1}], \\
\hat{G}_{\mu}^{a,b}(r) &= [G_{i-j}^{a,b}], & \hat{F}_{\mu}(r) &= [F_{i-j}].
\end{align*}
\]

(7)

where the indices \((i, j)\) run from 1 to \(r\), and the matrix elements \(G_{a,b}^n\) and \(F_n\) are given by Eqs. (6). Then, the Ising pair-field correlations like \(C_{\sigma\mu}^{ab}(r)\) reduce to \((2r) \times (2r)\) block-Toeplitz determinants:

\[
\begin{align*}
C_{\sigma\mu}^{ab}(r) &= \det \left[ \begin{array}{cc}
\hat{G}_{\sigma}^{ab}(r) & -\hat{F}_{\sigma}(r) \\
\hat{F}_{\mu}(r) & [\hat{G}_{\mu}^{ab}(r)]^T 
\end{array} \right], \\
C_{\mu\sigma}^{ab}(r) &= \det \left[ \begin{array}{cc}
\hat{G}_{\mu}^{ab}(r) & -\hat{F}_{\mu}(r) \\
\hat{F}_{\sigma}(r) & [\hat{G}_{\sigma}^{ab}(r)]^T 
\end{array} \right], \\
C_{\mu\mu}^{ab}(r) &= \det \left[ \begin{array}{cc}
\hat{G}_{\mu}^{ab}(r) & -\hat{F}_{\mu}(r) \\
\hat{F}_{\mu}(r) & [\hat{G}_{\mu}^{ab}(r)]^T 
\end{array} \right], \\
C_{\sigma\sigma}^{ab}(r) &= \det \left[ \begin{array}{cc}
\hat{G}_{\sigma}^{ab}(r) & -\hat{F}_{\sigma}(r) \\
\hat{F}_{\sigma}(r) & [\hat{G}_{\sigma}^{ab}(r)]^T 
\end{array} \right],
\end{align*}
\]

(8)

With all these provisions, the spin correlations are readily obtained. For the uniform part, \(S_i^j(n) = \langle I_i^n I_j^n \rangle\):

\[
\begin{align*}
S_i^a(r) &= \delta_{i0}[C_i^a(0) + C_i^a(0)] \\
&- 2C_i^a(0)C_i^a(0), \\
S_i^b(r) &= \delta_{i0}[C_i^b(0) + C_i^b(0)] \\
&- 2C_i^b(0)C_i^b(0), \\
S_i^\sigma(r) &= \frac{e^{ia \theta}}{2} [C_i^a(0)C_i^b(0) + C_i^b(0)C_i^a(0)].
\end{align*}
\]

(9)

Here \(C_i^a(0)\) are for the third (decoupled, off-critical) QIC. The extra terms in \(S_i^\sigma(r)\) is due to the admixture of the first two QICs in the presence of the magnetic field. Actually, \(4[C_3(0)]^2\) is the magnetization squared. For the staggered part, \(S_i^\sigma(n) = \langle N_i^n \rangle\):

\[
\begin{align*}
S_i^\sigma(r) &= C_{\mu\mu}^{ab}(r)C_{\mu}(r), \\
S_i^\mu(r) &= C_{\mu\mu}^{ab}(r)C_{\sigma}(r), \\
S_i^\tau(r) &= e^{i\alpha r}C_{\sigma}(r),
\end{align*}
\]

(10)

where \(C_{\sigma\mu}(r)\) are Ising correlations for the third decoupled QIC, which bear simple Toeplitz forms \((r \times r)\) matrices.

The fundamental and instructive quantity is the energy gap. The gap of the first two coupled QICs \((m\Delta-h)\) model is determined by \(\Delta^{ab\text{gap}} = \min(E_k^2)\). In axially symmetric case \((\Delta = 0)\), the gap decreases linearly:

\[
\Delta^{ab\text{gap}}(h) = (m - h)\theta(m - h).
\]

In general case, the gap function is shown in Fig. 4 (solid line), which has the following features: When \(h\) is small, it diminishes from \(m_2\) (the smaller mass of the two) as \(\Delta^{ab\text{gap}} \approx m_2 - \frac{h^2}{4}\). In the vicinity of the critical point, \(h_c = (m^2 - \Delta^2)^{1/2} = (m_1m_2)^{1/2}\), the gap vanishes linearly at both sides as \(\Delta^{ab\text{gap}} \approx \frac{h}{m}\). When the magnetic field is further increased to \(h^*_c \approx h_c + \frac{\Delta^2}{4m}\), the gap function in momentum space begins to shift from \(k = 0\) to \(k^*_c \approx \left(\frac{2m}{\Delta}\right)^{1/2} + \left(\frac{\Delta^2 + 2\Delta^4}{16m^2}\right)^{1/2} (h - h^*_c)^{1/2}\). As a result, a gapful incommensurate phase is expected at large \(h\). On the other hand, it is shown that when \(h > h^*_c\) and for small \(\Delta\), the gap \(\Delta^{ab\text{gap}} \approx \Delta\). Therefore, in the axially symmetric case, the gap closes in this region.
FIG. 1: The energy gap ($\Delta_{\text{gap}}$) of the coupled QICs ($m$-$\Delta$-$h$ model) as a function of $h$ (the solid line). The gap vanishes at $h_c = 0.0866025$ for $m = 0.1$ and $\Delta = 0.05$. Above $h_c$ ($=0.108080$), the dashed line is for the wavevector at which the gap locates. The (numerically extracted) solid circles represent the effective mass, $m_{\text{eff}}$, that governs all correlation functions; and the open circles are for the true incommensurate wavevector, $k^*_{\text{ab}}$, that enter the correlation functions in the incommensurate phase. The vertical dash-dotted line at $h^*_{\text{c}} = 0.098664$ is the true C-IC boundary. The wedge (dotted line) stuck to the $h_c$ point represents the effective mass, $m_{\text{eff}}$, at $h_c(m_1,m_2)$, arise from the trivial Ising lines ($m_1 = 0$ and $m_2 = 0$ at $h = 0$), and merge the C-IC sheets, pinned down by $h = h_{\text{c}}^*(m_1,m_2)$, at the U(1) symmetric line $h = m_1 = m_2$, i.e., the usual C-IC transition line in the axially symmetric case ($\Delta = 0$). Above the transition only the system with the U(1) symmetry is critical.

Unfortunately, although $\Delta_{\text{gap}}$ and $k^*_{\text{c}}$ are enlightening and analytically expressible, neither of them is the true quantity that controls the asymptotic behaviors of the correlation functions. We have to numerically extract the corresponding effective mass $m_{\text{eff}}$ (i.e., inverse of the correlation length) and effective incommensurate wavevector $k^*_{\text{ab}}$ from the fermion correlation functions, Eqs. (8), by evaluating the integrals. For comparison, we show these two quantities in the same Fig. 1 (the solid and open circles). As a result, the real C-IC transition point $h^*_{\text{c}}$ locates between $h_c$ and $h^*_{\text{c}}$. We also see from the figure that the effective mass, which is in general greater than the gap of the system, deviates significantly from the gap above the Ising transition. The mass grows rapidly unitil the system enters the incommensurate phase where the mass becomes field independent. In the vicinity of the Ising transition, the linearized effective mass (dotted wedge) asymptotically coincides with the numerical mass values (solid circles). The dissociation between the gap and mass is in fact due to the external field which breaks the Lorentz invariance of the model.

By combining Eqs. (5), (6), and (7), and the known values of functions $C_{\text{Is}}(r)$ and $C_{\text{IC}}(r)$, we compute the four correlation functions of the Ising pairs numerically. The parameter ranges for the $m$-$\Delta$-$h$ model are the same as in Fig. 1.
results are shown in Fig. 4. We find that below the Ising transition \( C^{ab}_{\mu\nu}(r) \), as in the \( h = 0 \) case, is asymptotically a constant, while above the transition \( C^{ab}_{\mu\nu}(r) \) becomes a constant. The lines decrease faster (in fact twice) in \( C^{ab}_{\mu\nu}(r) \) before the Ising transition and in \( C^{ab}_{\mu\nu}(r) \) after the transition. Furthermore, even in the incommensurate phase, functions \( C^{ab}_{\rho\mu}(r) \) and \( C^{ab}_{\mu\nu}(r) \) are not modulated by the wavevector \( k^*_c \). We also recognize that with respect to the effective Ising theory, the combined operators \( \mu_1 \sigma_2 \) and \( \mu_1 \mu_2 \) take effectively the roles of the Ising order and disorder fields across the transition, since their correlations have the standard power and exponential forms.

Finally, by Eqs. (9) and (10), we obtain the results of spin correlations in various phases. In the axially symmetric case \( (\Delta = 0) \), when the field exceeds the C-IC transition point, we find the transverse uniform spin correlations: \( S^I_0(r) \propto r^{-1}e^{-(m + 3)r} \) with the phase shift \( \delta(k_c) \approx k_c m \), and the incommensurate wavevector \( k_c \approx (2\pi/\eta)^{1/2}(h - m)^{1/2} \), and the longitudinal uniform spin correlations: \( \Delta S^I_1(r) = S^I_0(r) - M^2 \propto -r^{-2}[1 - \cos(2k_c r)] \) with \( M = k_c^2 \) the magnetization; and the transverse staggered correlations: \( \Delta S^y_{xy}(r) \propto r^{-1/2} \), and the longitudinal staggered correlations: \( \Delta S^z_{x}(r) \propto r^{-1}e^{-(m + 3)r} \cos(k_c r) \). These results are in agreement with those from other theories [9] just above the transition point. In anisotropic case, the asymptotics for the spin correlations are summarized in Table II. Here, the phase shifts in the incommensurate phase, restricted within \((0, \pi)\), are in general field and mass dependent; \( \eta < 1 \) is also a non-universal constant. As argued by Affleck [2], we verify that one of the transverse staggered spin correlations \( S^z_{xy} \) in our case) behaves simply like the correlation of an Ising variable across the transition, and the fluctuation of the longitudinal uniform correlation obeys the power-law \( \Delta S^z_{xy} \propto r^{-2} \) at the criticality.

To summarize, we have studied the Haldane spin-1 system with generic anisotropies under the effect of external magnetic field. We showed explicitly the Ising criticality in both the spectrum and correlation functions. The latter was calculated based on the establishment of the block-Toeplitz determinant representation for the correlations of the Ising pair-fields. A true long-range order is formed above the transition. We also found the incommensurability in high field is a rather robust property, which appears in both iso- and anisotropic systems, and the mass (not the gap) is field independent in the incommensurate phase. Finally, we emphasize the fact that the C-IC transition (point \( h_c^* \)) in the massive phase is thermodynamically unidentifiable, in other words, there is no anomaly associated with this transition in either magnetization or specific heat measurement. The discussions in this respect, as well as the detailed formalism of the present work, will be published elsewhere.

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\[ \text{Table I: Asymptotics of the uniform and staggered spin correlations when } \Delta > 0. \]

| \(| h = 0 \) | \(| 0 < h < h_c \) | \(| h = h_c \) | \(| h_c < h < h_c^* \) | \(| h > h_c^* \) |
|---|---|---|---|---|
| \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( \times \cos(k^*_c r + \delta^y) \) |
| \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( \times \cos(k^*_c r + \delta^y) \) |
| \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( \times \cos(k^*_c r + \delta^y) \) |
| \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( -r^{-1}e^{-(m + 3)r} \) | \( \times \cos(k^*_c r + \delta^y) \) |

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