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I analyze and comment on the following paper using bosonization technique. [Schulz PRB 1986, *Phase diagrams and correlations functions for quantum spin chains of arbitrary spin quantum number*]

I. GOAL AND SETTING OF THE PAPER

At the time when the paper was written, there was considerable discussions going on about the physical differences between integer and half-integer spin chains. Three years earlier, Haldane[2] had predicted gapless excitations for half-integer Heisenberg spin chains, while integer spins chains should only have gapped spinon excitations on top of a singlet ground state. Haldane used a mapping of the spin chain to the $O(3)$ non-linear sigma model and semi-classical quantization of the field theory. His arguments may have been regarded by many as rather heuristic and speculative; Schulz' paper has to be understood in the context of this ongoing controversy. It should be noted that many of Haldanes predictions were later found to be consistent with experiments on one-dimensional spin compounds.

The goal of the Schulz' paper is to attack the Heisenberg spin-S chain with a different approach than Haldane. With his approach, Schulz proposes to analyze the phase diagram and the correlation functions in detail. He claims that his findings confirm Haldanes predictions.

The idea of the Schulz' approach is to represent a spin $S = \frac{n}{2}$ chain by a n-legged spin-$\frac{1}{2}$ ladder. One can then attack the ladder problem starting from the single chain (i.e. supposing weak interchain coupling), using knowledge and techniques appropriate for spin-1/2 chains. First, Schulz applies the procedure to the spin-1 chain and discusses its phase diagram. He then generalizes to higher spins and discusses the correlation functions and phase diagrams.

II. SOME TECHNICAL DETAILS OF SECTION II

In the following I will discuss some of Schulz' results for the spin-1 chain. The Hamiltonian is given by

$$H = -\sum_i [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z] + D \sum_i (S_i^z)^2 \tag{1}$$

I will now rederive the bosonized expression for (1) given in Schulz' formulae (2.7) and (2.8). I first make the replacement $\boldsymbol{S}_i \to \boldsymbol{\sigma}_i + \boldsymbol{\tau}_i$. The resulting Hamiltonian in terms of the spin-1/2 operators σ and τ is:

$$H \to H' = -H_\sigma(J_z) - H_\tau(J_z) - H^\pm + H^z(J_z, D) + const. \tag{2}$$

where

$$\begin{aligned} H_\sigma(J_z) &= \sum_i \frac{1}{2}(\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+) + J_z\, \sigma_i^z \sigma_{i+1}^z & \text{(3a)} \\ H^\pm &= \sum_i \sigma_i^+ \tau_{i+1}^- + \tau_i^+ \sigma_{i+1}^- & \text{(3b)} \\ H^z(J_z, D) &= \sum_i 2D\, \sigma_i^z \tau_i^z - J_z(\sigma_i^z \tau_{i+1}^z + \tau_i^z \sigma_{i+1}^z) & \text{(3c)} \end{aligned}$$

To bring the Hamiltonian in a more conventional form, I stagger the x–y components of the spins by replacing $\sigma_i^\pm \to (-1)^i \sigma_i^\pm$ and $\tau_i^\pm \to (-1)^i \tau_i^\pm$. After this transformation, the Hamiltonian is

$$H' = H_\sigma(-J_z) + H_\tau(-J_z) + H^\pm + H^z(J_z, D) \tag{4}$$

H_σ and H_τ are conventional spin-1/2 chains. I will not bother to rederive the standard expressions for the bosonized spin-1/2 chain. One has just to be aware of the fact that Schulz uses the non-hermitian string operator when fermionizing the chain by Jordan-Wigner in his Eq. (2.1): $\sigma_i^+ = a_i^\dagger \exp(i\pi \sum_{j<i} a_j^\dagger a_j)$.

The expressions for the spins in terms of the bosonic fields can be found in Ref. 3, p. 167–168:[6]

$$\begin{aligned} \sigma^z(x) &= -\frac{1}{\pi}\partial\phi_1(x) + \frac{(-1)^x}{\pi}\cos(2\phi_1(x)) & \text{(5a)} \\ \sigma^+(x) &= \frac{1}{2\pi}\left\{(-1)^x e^{-i\theta_1(x)} + e^{-i\theta_1(x) - 2i\phi_1(x)}\right\} & \text{(5b)} \end{aligned}$$

and similar for spin τ with ϕ_1, θ_1 replaced by ϕ_2, θ_2, respectively.[7] Using formulae (5), I write the total spin to recover expressions (2.9) and (2.10) of Schulz:

$$\begin{aligned} S^+(x) &= (-1)^x \left(\sigma^+(x) + \tau^+(x)\right) \\ &= \frac{1}{2\pi}\left\{e^{-i\theta_1} + e^{-i\theta_2} + (-1)^x \left(e^{-i\theta_1 - 2i\phi_1} + e^{-i\theta_2 - 2i\phi_2}\right)\right\} \\ &= \frac{1}{\pi}\left\{e^{-iX_1/\sqrt{2}} \cos\left(X_2/\sqrt{2}\right) + (-1)^x e^{-i\left(X_1/\sqrt{2} + \sqrt{2}\psi_1\right)} \cos\left(X_2/\sqrt{2} + \sqrt{2}\psi_2\right)\right\} \end{aligned} \tag{6a}$$

$$\begin{aligned} S^z(x) &= \sigma^z(x) + \tau^z(x) \\ &= -\frac{1}{\pi}\partial\phi_1 + \frac{(-1)^x}{\pi}\cos(2\phi_1) + -\frac{1}{\pi}\partial\phi_2 + \frac{(-1)^x}{\pi}\cos(2\phi_2) \\ &= -\frac{\sqrt{2}}{\pi}\partial\psi_1 + (-1)^x \frac{2}{\pi}\cos\left(\sqrt{2}\psi_1\right)\cos\left(\sqrt{2}\psi_2\right) \end{aligned} \tag{6b}$$

where the following replacements have been made[8]

$$\begin{aligned} X_1(x) &= \frac{\theta_1(x) + \theta_2(x)}{\sqrt{2}}, \quad X_2(x) = \frac{\theta_1(x) - \theta_2(x)}{\sqrt{2}} \\ \psi_1(x) &= \frac{\phi_1(x) + \phi_2(x)}{\sqrt{2}}, \quad \psi_2(x) = \frac{\phi_1(x) - \phi_2(x)}{\sqrt{2}}\ . \end{aligned} \tag{7}$$

I can now immediately write down the bosonized Hamiltonian for $H_\sigma(-J_z)$ and $H_\tau(-J_z)$ in (4). The Luttinger parameters for the weakly anisotropic Heisenberg-1/2-chain can be found e.g. in Ref. 3, p. 166:

$$\begin{aligned} uK &= 1 \\ \frac{u}{K} &= 1 - \frac{4J_z}{\pi}\ . \end{aligned} \tag{8}$$

Using the replacement (7), the Luttinger part of the Hamiltonian is:

$$\begin{aligned} H_{Lutt} &= H_\sigma + H_\tau \\ &= \frac{1}{2\pi}\int dx \left\{(\partial\theta_1)^2 + (\partial\theta_2)^2 + (1 - \frac{4J_z}{\pi})\left((\partial\phi_1)^2 + (\partial\phi_2)^2\right)\right\} \\ &= \frac{1}{2\pi}\int dx \left\{(\partial X_1)^2 + (\partial X_2)^2 + (1 - \frac{4J_z}{\pi})\left((\partial\psi_1)^2 + (\partial\psi_2)^2\right)\right\}\ . \end{aligned} \tag{9}$$

Terms like $\cos(4\phi_i)$ are neglected by Schulz, because they are less relevant than the other perturbations to the Luttinger Hamiltonian.

For the expression of H^z, some care has to be taken in the continuous limit, regarding a sign change:

$$
\begin{aligned}
H^z &= \sum_i 2D\,\sigma_i^z\tau_i^z - J_z\,\left(\sigma_i^z\tau_{i+1}^z + \tau_i^z\sigma_{i+1}^z\right) \\
&\to \frac{1}{\pi^2}\int dx\,\{2D\,\left(-\partial\phi_1(x) + (-1)^x\cos 2\phi_1(x)\right)\left(-\partial\phi_2(x) + (-1)^x\cos 2\phi_2(x)\right) \\
&- J_z\big(-\partial\phi_1(x) + (-1)^x\cos 2\phi_1(x)\big)\left(-\partial\phi_2(x+1) + (-1)^{x+1}\cos 2\phi_2(x+1)\right) \\
&+ J_z\left(-\partial\phi_1(x+1) + (-1)^{x+1}\cos 2\phi_1(x+1)\right)\big(-\partial\phi_2(x) + (-1)^x\cos 2\phi_2(x)\big)\} \\
&\simeq \frac{2}{\pi^2}\int dx\,\{(D-J_z)\partial\phi_1\partial\phi_2 + (D+J_z)\cos 2\phi_1\cos 2\phi_2\} \\
&= \frac{1}{\pi^2}\int dx\,\{(D-J_z)\left((\partial\psi_1)^2 - (\partial\psi_2)^2\right) + (D+J_z)\left(\cos\sqrt{8}\psi_1 + \cos\sqrt{8}\psi_2\right)\}
\end{aligned}
\tag{10}
$$

Finally, $H^{\pm}$ is given by

$$
\begin{aligned}
H^{\pm} &= \sum_i \sigma_i^+\tau_{i+1}^- + \tau_i^+\sigma_{i+1}^- \\
&\to \frac{1}{(2\pi)^2}\int dx\,\{\left((-1)^x e^{-i\theta_1} + e^{-i\theta_1-2i\phi_1}\right)\left((-1)^{x+1}e^{-i\theta_2} + e^{-i\theta_2-2i\phi_2}\right) \\
&\quad + \left((-1)^x e^{-i\theta_2} + e^{-i\theta_2-2i\phi_2}\right)\left((-1)^{x+1}e^{-i\theta_1} + e^{-i\theta_1-2i\phi_1}\right)\} \\
&\simeq \frac{1}{(2\pi)^2}\int dx\,\{-e^{-i(\theta_1-\theta_2)} + e^{-i(\theta_1-\theta_2)-2i(\phi_1-\phi_2)} - e^{i(\theta_1-\theta_2)} + e^{i(\theta_1-\theta_2)-2i(\phi_1-\phi_2)}\} \\
&= \frac{2}{(2\pi)^2}\int dx\,\{-\cos(\theta_1-\theta_2) + \cos(\theta_1-\theta_2+2(\phi_1-\phi_2))\} \\
&= -\frac{1}{2\pi^2}\int dx\,\{\cos\sqrt{2}X_2 - \cos\left(\sqrt{2}X_2 + \sqrt{8}\psi_2\right)\}\ .
\end{aligned}
\tag{11}
$$

I have neglected rapidly oscillating terms in (10) and (11). The last term in the final expression of (11) is irrelevant and can be neglected. The total Hamiltonian can now be written as[9]

$$
\begin{aligned}
H' \to &\frac{1}{2\pi}\int dx\ \left\{(\partial X_1)^2 + (1 + 2(D-3J_z)/\pi)\,(\partial\psi_1)^2\right\} + \frac{1}{\pi^2}\int dx\ \cos\sqrt{8}\psi_1 \\
&+ \frac{1}{2\pi}\int dx\ \left\{(\partial X_2)^2 + (1 - 2(D+J_z)/\pi)\,(\partial\psi_2)^2\right\} + \frac{1}{\pi^2}\int dx\ \cos\sqrt{8}\psi_2 \\
&- \frac{1}{2\pi^2}\int dx\ \cos\sqrt{2}X_2 \\
&= H_1[X_1,\psi_1] + H_2[X_2,\psi_2]\ .
\end{aligned}
\tag{12}
$$

The representation of a spin-1 by two spin-1/2 is of course not exact. The space of two spin-1/2 is spanned by three triplet and one singlet state. The triplet sector can be mapped to the spin-1 space, so we neglected the singlet state. If the singlet state is sufficiently high in energy, it can indeed be neglected when considering ground state properties. Following the argumentation of Ref. 3, p. 190, a singlet-state on one site would annihilate the Heisenberg part of (1) at this site and thus cost the energy of order 1 with respect to the triplet states. This is very high in energy. It follows that the ground state must be composed of triplet states on each rung and the spin-1/2 representation is a reasonable approximation.

III. FINDINGS OF SECTION II

The main result of Section II is found in the discussion of the phase diagram of the spin-1 chain. First, Schulz observes that the Hamiltonian decouples to lowest order in the couplings into two independent and commuting parts $H_1[X_1, \psi_1]$ and $H_2[X_2, \psi_2]$, Eq. (12). Note that H_2 is quite a peculiar field theory, since it contains the integrated momentum: $\cos\left(\sqrt{2}X_2\left(x\right)\right) = \cos\left(\sqrt{2}\,\pi \int^x dx'\, \Pi\left(x'\right)\right)$. Schulz calls this a *vertex* or *disorder operator*, and distinguishes the phases depending if it is relevant or not. The main point is that the spectrum of H_2 is always massive, since at least one of the the mass generating operators $\cos\left(\sqrt{2}X_2\right)$ and $\cos\left(\sqrt{8}\psi_2\right)$ is always relevant (scaling dimension < 2). On the other hand, H_1 has 3 phases. For $3J_z - D > \pi/2$, the kinetic term in H_1 has a negative coefficient, and the field theory is ill-defined. Schulz conjectures that this phase should correspond to ferromagnetic order in the lattice problem. Second, there is a stripe of massless phase, where the potential term of H_1 is irrelevant. Finally, there is the massive phase of H_1 where the potential term is relevant.

The consequence of the previous observations for the diverse correlation functions is non-trivial, since the spin-1 operators are complicated superpositions of X_i and ψ_i (see Eqs. (6)). Schulz considers three correlation functions:

$$G_\perp(x) = \langle S^+(x)S^-(0)\rangle \tag{13a}$$

$$G_{\perp 2}(x) = \langle S^+(x)^2 S^-(0)^2\rangle \tag{13b}$$

$$G_z(x) = \langle S_z(x)S_z(0)\rangle \tag{13c}$$

Schulz finds a anti-ferro region where the staggered part of G_z has long-range order (H_1 massive, H_2 ordered); a singlet region, where all correlation functions decay exponentially (H_1 massive, H_2 disordered); the XY1-phase where the in-plain correlations $G_\perp$ and $G_{\perp 2}$

decay algebraically (H_1 massless, H_2 disordered); the XY2 phase where $G_\perp$ vanishes exponentially while $G_{2\perp}$ has long range algebraic dependency (H_1 massless, H_2 ordered).

Instead of repeating all arguments of Schulz, let me just point out one interesting feature in the phase diagram. In the region XY2, only correlations $(S^+)^2$ have algebraic decay, while correlations in S^+ decay exponentially. The physical reason for this is discussed by Schulz: The XY2 phase can only be reached with sufficiently large negative D. In the original spin-1 Hamiltonian (1), a negative D means that the singlet state $S^z = 0$ is frozen out, and the remaining Hamiltonian is effectively a spin-1/2 chain (massless). For this effective spin-1/2 problem, the raising operator $(S^+)^2$ is used, which is the reason for the algebraic decay of the correlation function $G_{\perp 2}$.

IV. SECTION III

The goal of Section III is to generalize the previous procedure to spin-S chains. Hopefully, one would find the phase diagram of spin chains with arbitrary spin.

Like before, the spin is decomposed into $2S$ half-spins at every site:

$$\boldsymbol{S} = \sum_{n=1}^{2S} \boldsymbol{\sigma}_n \tag{14}$$

The resulting spin-1/2 ladder is bosonized in a similar manner as previously. The resulting field theory contains $2S$ coupled boson fields ϕ_i. The Hamiltonian Schulz (3.4) is analogue to the spin-1 case:

$$\begin{aligned} H = & \frac{1}{2\pi} \int dx \left\{ (\pi \boldsymbol{\Pi})^2 + [1 - 2(D+J)/\pi] \, (\partial \boldsymbol{\phi})^2 + 2(D-J)/\pi \, \partial \boldsymbol{\phi}^T \bar{M} \partial \boldsymbol{\phi} \right\} \\ & + \frac{1}{\pi^2} \sum_{i<j} \int dx \left\{ \mu_1 \cos\left(2\left[\phi_i + \phi_j\right]\right) + \mu_2 \cos\left(2\left[\phi_i - \phi_j\right]\right) + \mu_3 \cos\left(\theta_i - \theta_j\right) \right\} \end{aligned} \tag{15}$$

where $\bar{M}$ is a matrix with all entries unity. The derivative term can be decoupled by means of the following unitary transformation:

$$\boldsymbol{\phi} = U \boldsymbol{\psi} \tag{16}$$

where

$$U_{mn} = \begin{cases} 1/\sqrt{2S} & , n = 1 \\ 1/\sqrt{(n-1)n} & , m < n > 1 \\ -\sqrt{(n-1)/n} & , m = n > 1 \\ 0 & , m > n > 1 \, . \end{cases} \tag{17}$$

A. Proof

Let me first show that the transformation is unitary:

$$A_{pq} = (U^T U)_{pq} = \sum_m U_{mp} U_{mq} \tag{18}$$

$$\begin{aligned} A_{11} &= \sum_m U_{m1}^2 = \frac{1}{2S} \sum 1 = 1 \\ A_{pp,\, p>1} &= \sum_m U_{mp}^2 = \sum_{m<p} \frac{1}{(p-1)p} + \frac{p-1}{p} = 1 \\ A_{pq,\, p<q} &= \sum_m U_{mp} U_{mq} = \sum_{m<p} U_{mp} U_{mq} + U_{pp} U_{pq} \\ &= \frac{1}{\sqrt{(p-1)p}} \frac{1}{\sqrt{(q-1)q}} \sum_{m<p} 1 - \sqrt{\frac{p-1}{p}} \frac{1}{\sqrt{(q-1)q}} = 0 \end{aligned} \tag{19}$$

which shows unitarity. Finally, I need to show that $\bar{M}$ is diagonalized:

$$(U^T \bar{M} U)_{pq} = \sum_{n,m} U_{np} M_{nm} U_{mq} = \sum_n U_{np} \sum_m U_{mq} = f_p f_q \, . \tag{20}$$

Clearly, I have

$$f_q = \sum_n U_{nq} = \begin{cases} \frac{1}{\sqrt{2S}} \sum 1 = \sqrt{2S} & , q = 1 \\ \sum_{n<q} \frac{1}{\sqrt{q(q-1)}} - \sqrt{\frac{q-1}{q}} = 0 & , q > 1 \end{cases} \tag{21}$$

which implies that

$$(U^T \bar{M} U)_{pq} = 2S \, \delta_{p1} \, \delta_{pq} \tag{22}$$

and concludes the proof.

The resulting Hamiltonian can be separated, similar to the spin-1 case, into a sine-Gordon system H_1 for $\psi_1 = \frac{1}{2S} \sum_n \phi_n$ and an order/disorder Hamiltonian H_2 for $\psi_n, n > 1$.

A draft of the spin-S phase diagram is thus very similar to the spin-1 case, containing the 5 regions:

- F: inapplicability of continuum limit.
- XY1: massless in-plain correlations.
- XY2: massless in-plain correlations to order $2S$.
- AF: massless Neel-order.
- S: all modes are massive; singlet phase.

However, the sine-Gordon-like term μ_1 contains all fields:

$$H_1^{int} \propto \mu_1 \sum_{i<j} \cos\left[2\phi_i + 2\phi_j\right] \ . \tag{23}$$

This fact gives rise to the important difference between integer and half-integer spin chains. Following his Equation (3.28), the author wants to illustrate this point. Consider the disordered region of H_2, where all $\psi_{n,n>1}$ decay exponentially. Potentially, the only massless term is ψ_1. The author argues that that one can always find combinations in the perturbative expansion in (23) to produce $\cos(\beta\,\psi_1)$. This fact is very important for the S^z correlation: The n-th order perturbation of this correlations is

$$\langle S^z(x)S^z(0)\rangle \simeq \mu_1^n \langle T\cos(2\phi(x))\cos(2\phi(0))\Pi_{q=1}^n \cos(2\phi_{i_q}(\bar{x}_q) + 2\phi_{j_q}(\bar{x}_q))\rangle \tag{24}$$

where T is time ordering and $\bar{x}$ represent integrated variables. The crucial point is that this correlation can always be arranged to produce the cosine of the sum of an *odd* number of ϕ_i. In case of half-integer spin, this means that we can arrange terms containing only $\cos(\beta\,\psi_1)$. At the same time, the perturbative expansion of the sine-Gordon operator itself will always contain at least one $\psi_{n,n>1}$; which makes this term irrelevant, i.e. ψ_1 is massless. As a result, one finds long-range AF order, and the singlet phase does not exist. In case of integer spin, the perturbative expansion of the S^z correlation always contains at least one $\psi_{n,n>1}$, so there is no order; this is the case in the singlet and $XY1$ phases found for spin-1.

In order to characterize the XY2 phase, Schulz considers the correlation

$$G_{\perp n} = \langle \left[S^+(x)\right]^n \left[S^-(0)\right]^n \rangle \ . \tag{25}$$

The XY2 phase is realized for large negative D, in the massless region of H_1. Following the same argument as in the spin-1 case, the intermediate S^z states of the original problem are frozen out, and $2S$ applications of S^+ connect the ground states. The resulting effective spin-1/2 problem is massless and results in algebraic decay of $G_{\perp n}$ for $n = 2S$.

V. TRANSVERSE CORRELATION

In Section IV, Schulz considers the phase $XY1$ which was found for both integer and half integer spin chains in the previous sections. In this phase, the fields Ψ_1, X_1 are massless, and are thus described by the Luttinger Hamiltonian. The transverse correlation is mainly given by $S^+ = c_\perp\, e^{-iX_1/\sqrt{2S}}$. The factor of proportionality $c_\perp$ involves the other, massive, fields. I will now derive Schulz' expression (4.8) for the transverse correlation. In the following, I will denote X_1 by θ.

Consider the massless Luttinger Field Theory. The quantity I want to calculate is

$$\begin{aligned} F(x,\tau) &= \langle T_\tau S^+(x,\tau) S^-(0,0)\rangle / c_\perp^2 \\ &= \langle T_\tau e^{-i\epsilon\theta(x,\tau)} e^{i\epsilon\theta(0,0)}\rangle = \frac{1}{Z_\theta}\int D\theta\, \overline{D\theta}\; e^{i\epsilon(\theta(0,0)-\theta(x,\tau))}\, e^{-S_\theta} \end{aligned} \tag{26}$$

since the only important contribution comes from θ, the other fields were integrated over in the last expression. The action for θ is given by ($u = 1$):

$$S_\theta = \frac{K}{2\pi}\int dx \int_0^\beta d\tau\, \{(\partial_\tau\theta)^2 + (\partial_x\theta)^2\} \tag{27}$$

The path integral is easily performed in Fourier space, where the action is diagonal:

$$S_\theta = \frac{K}{2\pi L\beta}\sum_{k,\omega_n}\{\omega_n^2 + k^2\}|\theta(k,n)|^2 = \boldsymbol{\theta}^\dagger M \boldsymbol{\theta} \tag{28}$$

with $M_{pq} = \delta_{pq}\,\frac{K}{2\pi L\beta}\,(\omega_p^2 + k_p^2)$. The exponent in (26) can be written as

$$i\epsilon(\theta(0,0) - \theta(x,\tau)) = \frac{i\epsilon}{L\beta}\sum_q (1 - e^{-iqr})\theta_q = i\left(\boldsymbol{J}^\dagger\boldsymbol{\theta} + \boldsymbol{\theta}^\dagger\boldsymbol{J}\right) \tag{29}$$

with $J_q = \frac{\epsilon}{2L\beta}(1 - e^{-iqr})$ and $qr = kx - \omega_n\tau$. After completing the square, I recover the usual formula for Gaussian integrals:

$$\frac{1}{Z_\theta}\int D\theta\,\overline{D\theta}\; e^{-\boldsymbol{\theta}^\dagger M\boldsymbol{\theta} + i(\boldsymbol{J}^\dagger\boldsymbol{\theta} + \boldsymbol{\theta}^\dagger\boldsymbol{J})} = e^{-\boldsymbol{J}^\dagger M^{-1}\boldsymbol{J}} \tag{30}$$

I need to evaluate the sum on the right hand side of (30):

$$\boldsymbol{J}^\dagger M^{-1}\boldsymbol{J} = \left(\frac{\epsilon}{2L\beta}\right)^2 \frac{2\pi L\beta}{K}\sum_{n\,k}\frac{2(1-cosqr)}{\omega_n^2+k^2} = \frac{\epsilon^2\pi}{K\beta L}\sum_{n\,k}\frac{1-cos(kx-\omega_n\tau)}{\omega_n^2+k^2} \tag{31}$$

The sum over the Matsubara frequencies $\omega_n = \frac{2\pi n}{\beta}$ can be performed using the residue theorem on the function multiplied by a Bose factor $n_B(z) = \frac{1}{e^{\beta z}-1}$:[10]

$$\begin{aligned} 0 = \frac{1}{2\pi i}\oint_{B(\infty)} d\omega\, n_B(\omega)\,\frac{1-cos(kx+i\omega\tau)}{-\omega^2+k^2} &= \frac{1}{\beta}\sum_n \frac{1-cos(kx-\omega_n\tau)}{\omega_n^2+k^2} \\ + n_B(k)\frac{1-\cos(kx+ik\tau)}{2k} &+ n_B(-k)\frac{1-\cos(kx-ik\tau)}{-2k}\ . \end{aligned} \tag{32}$$

Writing the sum over k as an integral $\frac{1}{L}\sum_k \to \frac{1}{2\pi}\int dk$, and adding the convergence factor $e^{-\alpha|k|}$, I get

$$\begin{aligned} &\frac{2\pi}{L\beta}\sum_{n\,k}\frac{1-cos(kx-\omega_n\tau)}{\omega_n^2+k^2} \\ &\quad = \int_{-\infty}^{\infty} dk\,[-n_B(k)\frac{1-\cos(kx+ik\tau)}{2k} + n_B(-k)\frac{1-\cos(kx-ik\tau)}{2k}]\ e^{-\alpha k} \\ &\quad = \int_0^\infty \frac{dk}{2k}\,(n_B(k)+n_B(-k))\,\{2-\cos(k(x+i\tau))-\cos(k(x-i\tau))\}\ e^{-\alpha k} \\ &\quad = \frac{1}{2}f(\frac{x-i\tau}{\beta},\frac{\alpha}{\beta}) + \frac{1}{2}f(\frac{x+i\tau}{\beta},\frac{\alpha}{\beta}) \end{aligned} \tag{33}$$

where

$$f(\xi,\delta) = \int_0^\infty \frac{dt}{t}\,\frac{e^t+1}{e^t-1}\,(1-\cos(t\xi))\,e^{-\delta t}\ . \tag{34}$$

To do this integral, I use the following relation [4, p. 249]

$$\log\Gamma(1+z) = \int_0^\infty \frac{dt}{t}\,\{z - \frac{1-e^{-zt}}{1-e^{-t}}\}\ . \tag{35}$$

Using this relation, I can write (34) in the following way:

$$f(\xi,\delta) = -\frac{1}{2}\log[\frac{\Gamma(1+i\xi+\delta)\Gamma(1-i\xi+\delta)\Gamma(i\xi+\delta)\Gamma(-i\xi+\delta)}{\Gamma(1+\delta)^2\,\Gamma(\delta)^2}] \tag{36}$$

Letting $\delta \to 0$ and using the following relation [4, p. 259]

$$|\Gamma(i\xi)|^2 = \frac{\pi}{\xi\sinh\pi\xi}\ , \tag{37}$$

I can write

$$f(\xi,\delta) = -\frac{1}{2}\log[\frac{\delta^2\,\pi^2}{\sinh^2\pi\xi}] = \log[\frac{\sinh\pi\xi}{\delta\,\pi}]\ . \tag{38}$$

Finally, using Eqs. (31), (33), and (38) I get

$$\begin{aligned} \boldsymbol{J}^\dagger M^{-1}\boldsymbol{J} &= \frac{\epsilon^2}{2K}\frac{1}{2}\{f(\frac{x-i\tau}{\beta},\frac{\alpha}{\beta})+f(\frac{x+i\tau}{\beta},\frac{\alpha}{\beta})\} \\ &= \frac{\epsilon^2}{4K}\log[\frac{\beta^2}{\alpha^2\pi^2}\sinh(\pi\frac{x-i\tau}{\beta})\sinh(\pi\frac{x+i\tau}{\beta})] \end{aligned} \tag{39}$$

and I recover Schulz' expression (4.7) :[11]

$$\begin{aligned} F(x,\tau) &= \langle Te^{-iX_1(x,\tau)/\sqrt{2S}}e^{iX_1(0,0)/\sqrt{2S}}\rangle = e^{-\boldsymbol{J}^\dagger M^{-1}\boldsymbol{J}} \\ &= (\alpha\pi T)^{2\xi}\{\sinh\pi T(x-i\tau)\,\sinh\pi T(x+i\tau)\}^{-\xi} \end{aligned} \tag{40}$$

with $\xi=\frac{\epsilon^2}{4K}=\frac{1}{8KS}$.

To get the transverse correlation, I need to Fourier transform the real time retarded correlation function $S_\perp$. This is done by Wick rotating $\tau\to it+\alpha\; sign(t)$. Using (26) and the fact that $t>0$, I get

$$S_\perp(x,t)=-iY(t)\langle[S^+(x,t),S^-(0,0)]|=Y(t)\,2\,c_\perp^2\,ImF(x,it) \tag{41}$$

It is clear from (40) that $F(x,it)$ has an imaginary part part only when $(x+t)(x-t)=x^2-t^2<0$, i.e. inside the light-cone. In this case I use the principal value of the exponent function: $(-a)^{-\xi}=e^{-\xi\,Log(-a)}=e^{-\xi\,(\ln a+i\pi)}=a^{-\xi}e^{-\xi i\,\pi}$. The Fourier transform can then be written as

$$\begin{aligned} &S_\perp(\omega,k) \\ &= -\sin(\pi\xi)\,2c_\perp^2\,(\alpha\pi T)^{2\xi}\int_{t,t^2-x^2>0}dx\,dt\,e^{i(\omega t-kx)}\,\{\sinh\pi T(x+t)\,\sinh\pi T(t-x)\}^{-\xi}\;. \end{aligned} \tag{42}$$

The integral is particularly simple using light-cone coordinates $\xi_\pm=t\pm x$:

$$S_\perp(\omega,t)=-\sin(\pi\xi)\,c_\perp^2\,(\alpha\pi T)^{2\xi}\,\Pi_\pm\int_0^\infty d\xi_\pm\,e^{i\xi_\pm(k\mp\omega)}\,(\sinh\pi T\xi_\pm)^{-\xi} \tag{43}$$

To evaluate the integral $\int_0^\infty ds\,e^{i\,sq}\,(\sinh\pi T\,s)^{-s}$, I use Eulers first integral, which is defined as $B(x,y)=\int_0^1 dt\,t^{x-1}\,(1-t)^{y-1}$. I perform the variable change $t^{1/2}=e^{-\pi T\,s}$:

$$\begin{aligned} \int_0^\infty ds\,e^{i\,sq}\,(\sinh\pi Ts)^{-\xi} &= 2^\xi\int_0^1\frac{dt}{2\pi T\,t}\,t^{-iq/(2\pi T)}\,(t^{-1/2}-t^{1/2})^{-\xi} \\ &= \frac{2^\xi}{2\pi T}\int_0^1 dt\,t^{-i\,q/(2\pi T)-1}\,t^{\xi/2}(1-t)^{-\xi} \\ &= \frac{2^\xi}{2\pi T}\,B(-\frac{i\,q}{2\pi T}+\frac{\xi}{2},1-\xi) \end{aligned} \tag{44}$$

Finally, the transverse correlation (43) can be written as

$$S_\perp(k,\omega) = -c_\perp^2 \sin(\pi\xi)\, \alpha^2 (2\pi T)^{2(\xi-1)}\; B(\frac{k-\omega}{2\pi i T} + \frac{\xi}{2}, 1-\xi)\; B(\frac{k+\omega}{2\pi i T} + \frac{\xi}{2}, 1-\xi) \qquad (45)$$

which is Schulz' expression (4.8).

The imaginary part of the spin susceptibility, $S(k,\omega) = Im\chi$, (longitudinal or transverse correlation) has the physical meaning of the spectral weight of spin excitations. It can be measured in neutron scattering experiments, where it is proportional to the scattering cross section. It is interesting to note that the $S_\perp$ here has no singularities on the real axis, as it would be the case for a Fermi-liuid on the quasi-particle dispersion.

VI. CONCLUSIONS

For integer spin chains, Schulz finds a region in the phase space with singlet ground state and massive excitations. For half-integer spin chains, this region is absent. Instead of the singlet phase, Schulz finds a massive anti-ferro region. The massless $XY1$ region, however, is enhanced in the half-integer case. In both cases, there are the $XY1$ and $XY2$ phases, where transverse and higher power transverse correlations, respectively, have algebraic decay.

The primary goal of the paper was to confirm Haldanes predictions. As far as I can see, Schulz predicts a much more sophisticated and detailed phase diagram than Haldane did. Haldane predicted a massive magnon in the integer case. While in the half-integer case, Haldane predicts additionally gapless excitations.

One important shortcoming of Schulz procedure is that it is a weak coupling approach. Higher order terms will couple the fields of H_1 and H_2 and make a treatment much more difficult.

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[1] H. J. Schulz, Phys. Rev. B 34, 6372 (1986).

[2] F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983); F. D. M. Haldane, Phys. Lett. 93A, 464 (1983).

[3] T. Giamarchi, *Quantum Physics in One Dimension*, Clarendon Press, Oxford.

[4] Whittaker & Watson, *A Course of Modern Analysis*, 4th edition, Cambridge University Press.

[5] V. J. Emery, *Highly Conducting One-Dimensional solids*, Plenum, New York 1979.

[6] In fact, in Ref. 3, Eq. (6.35), there is an additional factor of $\sqrt{2\pi}$ for σ^+. Using this factor, I cannot reproduce Schulz' expression (2.9) and (2.10). The reason may be that Schulz uses the asymetric definition of the Fourier transform.

[7] I will always set the lattice spacing a to unity, when it does not lead to confusion.

[8] To get Schulz (2.9) from Eq. (6b), I have to assume that ϕ and θ commute at the same point, i.e. $[\theta(x), \phi(x)] = 0$.

[9] The factor $-\frac{1}{2}$ in $H^{\pm}$ disagrees with the expression of Schulz, who finds -1 instead. I have not found where this discrepancy comes from. Maybe I employ the bosonization formulas too naively. This numerical factor, however, does not enter Schulz' following discussion of the spin-1 chain phase diagram.

[10] There is a subtlety here which I do not full understand. For truly imaginary time ($|Re(\tau)| > \alpha$), the integrand $\cos(kx - i\omega\tau)$ will diverge exponentially as $Re(\omega) \to \infty$. For $Re(\omega) > 0$, this divergency is cut off by the Bose factor as long as $Re(\tau) < \beta$. However, this this does not work in the half-plane $Re(\omega) < 0$ since the Bose factor goes to -1 in this directions. Nevertheless, the integral is well behaved in real time where $|Re(\tau)| < \alpha$.

[11] Note that I do not get the intermediate relation Schulz (4.4) for the correlation, which he claims to be exact for arbitrary α. With the method I use here, the limit $\alpha \to 0$ has to be taken earlier in order to apply relation (37).

APPENDIX A: ORIGINAL TASK

Read and comment the paper “Phase diagrams and correlation exponents for quantum spin chains of arbitrary spin quantum number” PRB 34 6372 (1986) by H. J. Schulz. Here are some questions to guide your comments, but feel free to add any comment you want.

- What is the goal of this paper ? What was the main debate that the paper is trying to address at the time it was written ?
- Do you agree with the representation of spin 1 operators used at the beginning of Section II ? What is the difference with a real spin 1 ? Is this difference important ?
- Rederive yourself the Hamiltonian (2.7), (2.8) and the spin operators (2.9), (2.10), using the bosonization technique.
- What are the main findings of section II ?
- What is the goal of Section III ?
- Show that (3.9) is indeed a correct unitary transformation to diagonalize the bilinear part of (3.4).
- What does the author want to show following equation (3.28) ?
- Rederive formula (4.8). What is this quantity representing in physical terms ? How can it be measured ?
- Did the paper reach the goals it sets in the introduction ? Other comments on this paper ?