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# Exact Haldane mapping for all $S$ and super universality in spin chains

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**Abstract** – The low-energy dynamics of the anti-ferromagnetic Heisenberg spin  $S$  chain in the semiclassical limit  $S \rightarrow \infty$  is known to map onto the  $O(3)$  nonlinear  $\sigma$ -model with a  $\theta$  term in  $1+1$  dimension. Guided by the underlying dual symmetry of the spin chain, as well as by the recently established topological significance of “dangling edge spins”, we report an *exact* mapping onto the  $O(3)$  model that avoids the conventional large- $S$  approximation altogether. Our new methodology demonstrates all the super universal features of the  $\theta$ -angle concept that previously arose in the theory of the quantum Hall effect. It explains why Haldane’s original ideas remarkably yield the correct answer in spite of the fundamental complications that generally exist in the idea of semiclassical expansions.

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In 1983, Haldane proposed that the low-energy dynamics of the anti-ferromagnetic Heisenberg spin  $S$  chain can be taken from the  $O(3)$  nonlinear  $\sigma$ -model (NLSM) in  $1+1$  dimension and in the presence of the  $\theta$  term [1]. At least within the limitations of a large- $S$  approximation the parameter  $\theta$  was found to take on the values 0 or  $\pi$  only, depending on whether  $S$  is integral or half-integral, respectively. Since the standard  $O(3)$  model with  $\theta = 0$  is known to display a mass gap [2], Haldane concluded that the integral spin chain is always gapped. This is unlike the  $S = 1/2$  chain, for example, which from the Bethe ansatz solution is known to display gapless excitations [3]. Based on numerical work it is now generally accepted that the uniform integral spin chain is always gapped, whereas the half-integral spin chain is generally gapless.

It has recently been pointed out, however, that a universal topological feature of the  $\theta$ -angle concept has historically been overlooked [4]. The  $\theta$ -vacuum quite generally displays *massless chiral edge excitations* [5] that have important consequences for the theory on the strong-coupling side. Within the Grassmannian  $U(M+N)/U(M) \times U(N)$  nonlinear sigma model

approach to localization and interaction phenomena, for example, it was shown that the massless edge excitations are directly related to the existence of *robust topological quantum numbers* that explain the stability and precision of the quantum Hall effect [6]. This has led to the idea of *super universality* of quantum Hall physics that, unlike the common belief in the field, is independent of the details of the theory such as the number of field components and in particular, the replica limit  $M, N \rightarrow 0$  [6].

Based on the Haldane mapping it is next natural to expect that the super-universality statement can be extended to also include quantum spin liquids. Indeed, renormalization group studies have clearly indicated that the dimerised  $S = 1/2$  spin chain displays all the basic features of the quantum Hall effect [4] in much the same manner as what has recently been observed, for example, in the exactly solvable large- $N$  limit of the  $CP^{N-1}$  model [7]. The dynamics of the *dangling edge spins* of the chain thereby plays a role that is in many ways the same as that of the *massless chiral edge excitations* of the  $\theta$ -vacuum. Unfortunately, a generalized Haldane mapping that includes the dangling spins at the edges of the spin  $S$  chain has so far been obtained only for the semiclassical  $S = \infty$  limit [4]. Given the extensive literature on the subject of quantum spin chains, it is somewhat surprising to know that not a single attempt has been reported that

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would in principle resolve this longstanding drawback and extend the Haldane mapping to include finite values of  $S$ .

One of the main objectives of the present letter is to show that the statement of super universality of quantum spin liquids cannot in general be established by using the semiclassical large- $S$  idea alone. To illustrate the problems we first recall the Hamiltonian of the spin chain

$$\mathcal{H} = \frac{J}{S} \sum_I (\mathbf{S}_{I1} \cdot \mathbf{S}_{I2} + \kappa \mathbf{S}_{I2} \cdot \mathbf{S}_{I+11}). \quad (1)$$

Here,  $J > 0$  favors the anti-ferromagnetic (Néel) ordering, the integer  $I$  is the dimer index and the subscripts 1 and 2 denote the two sites within each dimer. The variable  $\kappa$  with  $0 < \kappa < \infty$  is the dimensionless nearest-neighbor coupling between the dimers. The path integral representation involves  $O(3)$  vectors  $\hat{\mathbf{n}}(t)$  with  $\hat{\mathbf{n}}^2 = 1$  and  $t$  denoting the imaginary time. The action is [8]

$$\begin{aligned} \mathcal{S} = & iS \sum_I \Omega[\hat{\mathbf{n}}_{I1}] + \Omega[\hat{\mathbf{n}}_{I2}] \\ & + SJ \sum_I \oint (\hat{\mathbf{n}}_{I1} \cdot \hat{\mathbf{n}}_{I2} + \kappa \hat{\mathbf{n}}_{I2} \cdot \hat{\mathbf{n}}_{I+11}). \end{aligned} \quad (2)$$

The quantity  $\Omega[\hat{\mathbf{n}}_{I\alpha}]$  is the solid-angle term associated with each lattice site  $I\alpha$  and  $\oint = \int_0^\beta dt$ . To extract the low-energy dynamics of the spin chain from eq. (2) several basic assumptions are necessary. The historical procedure was based on the change of variables [9]

$$\mathbf{m}_I = \frac{1}{2}(\hat{\mathbf{n}}_{I1} - \hat{\mathbf{n}}_{I2}), \quad \mathbf{l}_I = \frac{1}{2}(\hat{\mathbf{n}}_{I1} + \hat{\mathbf{n}}_{I2}), \quad (3)$$

where  $\hat{\mathbf{m}}_I = \mathbf{m}_I/|\mathbf{m}_I|$ , which is a measure of the Néel ordering, is taken as the *soft mode* in the problem that should be retained. The field variable  $\mathbf{l}_I$ , on the other hand, is taken as the *hard mode* that should be integrated out. The simplest way to do this is by using semiclassical approximations. Assuming  $S \rightarrow \infty$  then eq. (2) can be evaluated at the saddle point which in the long-wavelength limit (slowly varying  $\hat{\mathbf{m}}_I$ ) yields the NLSM in the presence of the  $\theta$ -angle [4,9]. The complications, however, occur in the computation of the  $1/S$  corrections that all diverge as  $\beta \rightarrow \infty$ . The origin of the divergences is easily understood from the following *exact* expression for the solid-angle term of each dimer [10]:

$$\Omega[\hat{\mathbf{n}}_{I1}] + \Omega[\hat{\mathbf{n}}_{I2}] = 2 \oint \mathbf{l}_I \cdot \hat{\mathbf{m}}_I \times \partial_t \hat{\mathbf{m}}_I. \quad (4)$$

The action of the “hard” modes has therefore no time derivatives and this, in turn, implies that *coincident* operators  $\mathbf{l}_I(t)$  have a divergent expectation value. What this simple example is telling us is that semiclassical expansions are quite generally plagued by ambiguities that are inherent in the bosonic path integral representation of eq. (2). These ambiguities, as we shall see later on in this letter, are the main reason why the general theory of the Heisenberg anti-ferromagnet has not advanced beyond the naive  $S = \infty$  saddle point limit.

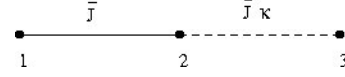


Fig. 1: The 3-spin problem with relative bond strengths 1 and  $\kappa$ .

**Three-spin problem.** – As the most important step next we introduce a novel mapping onto the NLSM that avoids the use of semiclassical approximations altogether. This is accomplished if, instead of eq. (3), we pursue an effective action of the spin chain as defined by *decimation*, *i.e.* by eliminating the spins on one sublattice (say,  $\hat{\mathbf{n}}_{I1}$ ) while retaining those on the other ( $\hat{\mathbf{n}}_{I2}$ ). The primary focus will be on *open* spin chains containing  $2N + 1$  sites since they display both the subtleties of “dangling edge spins” and “dual invariance.” By dual invariance we mean that the dimerised spin system described by eqs. (1) and (2) is invariant under the interchange between the weak and strong bonds

$$J \rightarrow J\kappa, \quad \kappa \rightarrow \frac{1}{\kappa}. \quad (5)$$

For simplicity we first consider the three-spin system as sketched in fig. 1 which is the simplest possible system with edges that is manifestly self-dual. It is advantageous to express the  $O(3)$  vector field  $\hat{\mathbf{n}}$  in terms of a Grassmannian field variable  $Q = \hat{\mathbf{n}} \cdot \boldsymbol{\tau} \in SU(2)/U(1)$ , with  $\boldsymbol{\tau}$  denoting the Pauli matrices. This leads to the three-spin action

$$\begin{aligned} \mathcal{S}[Q_1, Q_2, Q_3] = & iS \left\{ \Omega[Q_1] + \Omega[Q_2] + \Omega[Q_3] \right\} \\ & + \frac{1}{2} SJ \oint \text{tr}(Q_1 + \kappa Q_3) Q_2. \end{aligned} \quad (6)$$

We can always write  $Q = T^{-1} \tau_z T$  with  $T \in SU(2)$  such that the solid-angle term can be expressed explicitly according to  $i\Omega[Q] = i\Omega[T] = \oint \text{tr} T \partial_t T^{-1} \tau_z$  [4]. The decimation of the three-spin system is defined as follows:

$$e^{-\mathcal{S}_{eff}[Q_1, Q_3]} = \int \mathcal{D}[Q_2] e^{-\mathcal{S}[Q_1, Q_2, Q_3]}. \quad (7)$$

To evaluate  $\mathcal{S}_{eff}$  we notice that the matrix  $Q_1 + \kappa Q_3$  in eq. (6) is Hermitian and traceless. Therefore, let us write

$$J(Q_1 + \kappa Q_3) = BV^{-1} \tau_z V, \quad (8)$$

$$B = J(1 + \kappa) \sqrt{1 - \frac{\kappa}{2(1 + \kappa)^2} \text{tr} \delta Q \delta Q}, \quad (9)$$

where  $V \in SU(2)$  and  $\delta Q = Q_3 - Q_1$  which is taken as a small quantity. Similarly, we expand the matrix  $V$  in powers of the differential  $\delta T = T_3 - T_1$ ,

$$V = T_1 + \frac{\kappa}{1 + \kappa} \delta T + \mathcal{O}(\delta^2). \quad (10)$$

Based on eqs. (8)–(10) we obtain  $\mathcal{S}_{eff}$  order by order in a derivative expansion. To see this we replace

$Q_2 \rightarrow V^{-1}Q_2V$  such that eq. (6) can be rewritten as

$$S = iS(\Omega[T_1] + \Omega[T_3]) + \mathcal{S}_0[Q_2] + \tilde{S}[Q_1, Q_2, Q_3], \quad (11)$$

$$\mathcal{S}_0[Q_2] = S \oint \text{tr} \left( T_2 \partial_t T_2^{-1} + \frac{B_0}{2} Q_2 \right) \tau_z, \quad (12)$$

$$\tilde{S}[Q_1, Q_2, Q_3] = S \oint \text{tr} \left( V \partial_t V^{-1} + \frac{\delta B}{2} \tau_z \right) Q_2 \quad (13)$$

with  $B_0 = J(1 + \kappa)$  and  $\delta B = B - B_0$ . Notice that the piece  $\mathcal{S}_0$  in eqs. (11) and (12) is the action of a single spin  $S$  in a constant magnetic field  $B_0$  which is *exactly* solvable. Of interest are the non-vanishing one- and two-point correlations of the  $Q_2 = Q_2^{\sigma\sigma'}$  matrix field [4,5],

$$\langle Q_2 \rangle = -\tau_z, \quad \langle Q_2^{21}(0) Q_2^{12}(t) \rangle = \frac{2}{S} \vartheta(t) e^{-B_0 t}. \quad (14)$$

Here, the limit  $\beta \rightarrow \infty$  ( $\beta$  being the inverse temperature) is understood and  $\vartheta(t)$  denotes the Heaviside step function. The piece  $\tilde{S}$  in eqs. (11) and (13) contains derivatives acting on the “soft” modes  $Q_1$  and  $Q_3$  and can be treated in a cumulant expansion. This leads to  $\mathcal{S}_{eff}$  obtained to lowest orders in  $\partial_t$  and  $\delta$ ,

$$\begin{aligned} \mathcal{S}_{eff}[Q_1, Q_3] &= iS\Omega[T_3] + S \frac{\kappa}{\kappa+1} \\ &\times \oint \text{tr} \left\{ \frac{J}{4} (\delta Q)^2 + \frac{1}{J\kappa} (\partial_t Q)^2 - \delta(T \partial_t T^{-1} \tau_z) \right\}. \end{aligned} \quad (15)$$

**Exact mapping.** – Equation (15) can be directly generalized to obtain the effective action  $\mathcal{S}_{exact}^o$  for the dimerised spin chain with  $2N + 1$  sites and the result is

$$\begin{aligned} \mathcal{S}_{exact}^o &= \sum_{m=1}^N \left\{ \mathcal{S}_{eff}[Q_{2m-1}, Q_{2m+1}] - iS \Omega[T_{2m+1}] \right\} \\ &+ iS \Omega[T_{2N+1}]. \end{aligned} \quad (16)$$

In the continuum limit we obtain the NLSM,

$$\begin{aligned} \mathcal{S}_{exact}^o &= \frac{1}{g} \int \text{tr} \left\{ \frac{1}{c} (\partial_t Q)^2 + c (\partial_x Q)^2 \right\} + i\theta \mathcal{C}[Q] \\ &+ iS \Omega[T(L)]. \end{aligned} \quad (17)$$

Here,  $\int$  denotes the space-time integral  $\oint dt \int_0^L dx$ ,  $L = 2Na$  with  $a$  the lattice constant.  $\mathcal{C}[Q]$  is the *topological charge* of the matrix field  $Q$ ,

$$\mathcal{C}[Q] = \frac{1}{16\pi i} \int \text{tr} \epsilon_{\mu\nu} Q \partial_\mu Q \partial_\nu Q = \frac{\Omega[T(0)] - \Omega[T(L)]}{4\pi} \quad (18)$$

and the NLSM parameters are given by<sup>1</sup>

$$\theta(\kappa) = 4\pi S \frac{\kappa}{1 + \kappa}, \quad g(\kappa) = \frac{1 + \kappa}{S\sqrt{\kappa}}, \quad c(J, \kappa) = aJ\sqrt{\kappa}. \quad (19)$$

We will next employ these results to draw important conclusions that are valid for arbitrary values of  $S$ .

<sup>1</sup>As explained later in the text the same expressions are obtained in the naive  $S = \infty$  approximation [4,9].

**Duality and super universality.** – The solid-angle term in eq. (17) is clearly the action of a single “edge spin” that makes all the difference between an *open* spin chain and *closed* one. In anticipation of the fact that the “bulk” of the system is periodic in the “angle”  $\theta$  we write

$$\theta(\kappa) = \theta_B(\kappa) + 2\pi k(\kappa), \quad (20)$$

where  $-\pi < \theta_B(\kappa) \leq \pi$  denotes the *fractional* piece and  $k(\kappa) = 0, 1, \dots, 2S$  the *integral* piece of  $\theta(\kappa)$ . Notice that under the transformation of eq. (5), the NLSM parameters are replaced by

$$\begin{aligned} \theta_B(1/\kappa) &= -\theta_B(\kappa), & k(1/\kappa) &= S - k(\kappa), \\ g(1/\kappa) &= g(\kappa), & c(J\kappa, 1/\kappa) &= c(J, \kappa). \end{aligned} \quad (21)$$

Equation (20) therefore permits a splitting of eq. (17) into a “bulk” part  $\mathcal{S}_B[Q]$  and an “edge” part  $\mathcal{S}_E^o[T]$  that are decoupled under the dual transformation. Specifically, we rewrite

$$\mathcal{S}_{exact}^o = \mathcal{S}_B[Q] + \mathcal{S}_E^o[T], \quad (22)$$

$$\mathcal{S}_B[Q] = \frac{1}{g} \int \text{tr} \left\{ \frac{1}{c} (\partial_t Q)^2 + c (\partial_x Q)^2 \right\} + i\theta_B \mathcal{C}[Q], \quad (23)$$

$$\mathcal{S}_E^o[T] = i \frac{k}{2} \Omega[T(0)] + i \left( S - \frac{k}{2} \right) \Omega[T(L)]. \quad (24)$$

These final expressions are the principal results of this letter. Notice that eq. (24) is a fundamental statement made on the “edge” of the  $\theta$ -vacuum that has traditionally gone unnoticed [4,6]. Following eqs. (12) and (14) it is the *critical* action of “dangling edge spins” and should therefore be regarded as an integral part of the low-energy dynamics of the spin chain [11]. To understand this aspect of the problem we first consider the class of topological field configurations  $Q_0$  for which  $\mathcal{C}[Q_0]$  is strictly an integer. As is well known, this class sets the stage for the “instanton picture” of the  $\theta$ -angle and is geometrically defined by identifying the edge as a single point, *i.e.*  $Q_0$  is a constant matrix along the edge of the system, say  $Q_0 = \tau_z$  [6]. The action for the edge equation (24) is now a trivial phase factor and we immediately recognize  $\mathcal{S}_{exact}^o = \mathcal{S}_B[Q_0]$  as the theory of the “bulk” of the system that only depends on  $\theta(\kappa)$  modulo  $2\pi$ .

To incorporate the edge excitations we write  $Q = U^{-1}Q_0U$ . Here  $U \in SU(2)$  represents the “fluctuations” about the boundary condition  $Q_0 = \tau_z$  that carry a *fractional* topological charge. Discarding unimportant phase factors eq. (24) now reads  $\mathcal{S}_E^o[T] = \mathcal{S}_E^o[U]$  indicating that the matrix  $U$  is the basic field variable for the “edge.” Of primary interest is the effective action for “edge” excitations  $\tilde{\mathcal{S}}_E^o[U]$  which is given by [4,6]

$$e^{-\tilde{\mathcal{S}}_E^o[U]} = e^{-\mathcal{S}_E^o[U]} \int_{\partial V} \mathcal{D}[Q_0] e^{-\mathcal{S}_B[U^{-1}Q_0U]}. \quad (25)$$

Here,  $\partial V$  reminds us of the boundary condition  $Q_0 = \tau_z$ . Next, we make use of the fact that the two-dimensional

theory of eq. (23) develops a *mass gap* when  $\theta_B(\kappa) \approx 0$  or  $\theta(\kappa) \approx 2\pi k(\nu)$  [2]. A finite mass gap in the “bulk” means that the functional integral of eq. (25) is insensitive to changes in the boundary conditions and, hence,  $\mathcal{S}_E^o[U] \equiv \mathcal{S}_E^o[U]$  except for  $U$ -independent terms. We therefore conclude that the dimerised spin chain with varying values of  $\kappa$  displays  $2S + 1$  different topological phases, labelled by the integer  $k(\kappa)$ , where the low-energy excitations are solely those of the “dangling edge spins” with quantum numbers  $k(\kappa)/2$  and  $S - k(\kappa)/2$ , respectively. These phases must in general be separated by *quantum phase transitions* (or a vanishing mass gap in the bulk) occurring at intermediate values of  $\kappa$  where  $\theta_B(\kappa)$  makes a “jump” from  $+\pi$  to  $-\pi$ . Notice that gapless excitations are in general necessary in order for the spin chain to be able to *transport* a spin- $\frac{1}{2}$  quantum over *macroscopic* distances from one edge to the other. Moreover, in complete analogy with the “electrodynamics picture” of the  $\theta$ -angle [12] one may interpret the “jump” in  $\theta_B(\kappa)$  in terms of the creation of “Coleman charges” that move to the opposite edges so as to maximally shield the “background electric field”  $\theta(\kappa)$  (see footnote <sup>2</sup>).

In summary, emerging from eqs. (22)–(25) are precisely the *super universal* features of the  $\theta$ -vacuum concept that have previously been discovered in the context of the quantum Hall effect [6]. The statement of super universality becomes all the more transparent when, for example, the “dangling edge spins” are identified with the phenomenon of *massless chiral edge excitations*, the spin chain parameter  $\theta(\kappa)/2\pi$  is replaced by the *filling fraction* of the Landau levels and, finally, the integer  $k(\kappa)$  is recognized as the *robustly quantized* Hall conductance [4]. For completeness we list the results for eq. (24) for *open* spin chains ( $\mathcal{S}_E^e$ ) and *closed* ones  $\mathcal{S}_E^p$  that contain an *even* number of sites,

$$\mathcal{S}_E^e[U] = i\frac{k}{2} \left\{ \Omega[U(0)] - \Omega[U(L)] \right\}, \quad \mathcal{S}_E^p[U] = 0. \quad (26)$$

**Semiclassical theory.** – Next, it is of interest to know what our explicit and exact results teach us about the problem of semiclassical expansions that to date has spanned the subject. For this purpose we address the single-spin problem of eq. (12) and employ the Schwinger boson representation  $Q_2^{\sigma\sigma'} = \delta_{\sigma\sigma'} - 2z_\sigma z_{\sigma'}^*$ , with  $\mathbf{z}^* \cdot \mathbf{z} = 1$ . Fixing the  $U(1)$  gauge such that  $z_1 = z_1^* = \sqrt{1 - z_2^* z_2}$ , the  $Q_2$  matrix field can be written as

$$Q_2 = - \begin{pmatrix} 1 - 2z_2^* z_2 & 2z_2 \sqrt{1 - z_2^* z_2} \\ 2z_2^* \sqrt{1 - z_2^* z_2} & -1 + 2z_2^* z_2 \end{pmatrix}. \quad (27)$$

<sup>2</sup>Coleman’s charges are distinctly different from the massless edge excitations that fundamentally explain the quantum Hall effect. As explained in the text, these edge excitations are a previously unrecognized universal feature of the  $\theta$ -angle concept that resolves, amongst many other things, the longstanding conflicts between “large- $N$  picture” and the “instanton picture,” see, *e.g.*, [7].

The single-spin action of eq. (12) becomes simply

$$\mathcal{S}_0 = 2S \oint \left\{ z_2^*(t) \partial_t z_2(t) + B_0 z_2^*(t - \epsilon) z_2(t) \right\}. \quad (28)$$

For reasons to be explained shortly, we have introduced an infinitesimal *time-splitting* quantity  $\epsilon > 0$  in the definition of  $\mathcal{S}_0$ . In the large- $S$  limit the propagator becomes

$$\langle z_2^*(0) z_2(t) \rangle = \frac{1}{2S} \vartheta(t - \epsilon) e^{-B_0 t}. \quad (29)$$

It can be shown that eqs. (27)–(29) are completely equivalent to the Holstein-Primakoff representation of the single spin. The effect of our introduction of the time-splitting quantity  $\epsilon$  in eqs. (28) and (29) is to render the expectation value of *coincident* operators identically equal to zero. The remarkable conclusion that one can draw from all this is that the exact correlations of eq. (14) are obtained in the limit  $S \rightarrow \infty$  and the corrections are zero to all orders in  $1/S$  [13].

The subtle but crucial feature of *coincident* operators is generally lost in eqs. (2) and (12), a drawback of the bosonic path integral that explains why the traditional saddle point or large- $S$  technique is complicated. On the other hand, the present theory fundamentally resolves these ambiguities since our exact and semiclassical results can be compared directly with the knowledge obtained from different sources, notably the Hamiltonian formalism. Finally, our methodology is not specifically designed for  $SU(2)$  spins alone. It can also be applied to the  $SU(n)$  case, for example, as well as to the Heisenberg anti-ferromagnet in higher dimensions [14].

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