Exact and simple results for the XYZ and strongly interacting fermion chains

Paul Fendley and Christian Hagendorf

Department of Physics, University of Virginia, Charlottesville, VA 22904-4714, USA

E-mail: fendley@virginia.edu

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Abstract
We conjecture exact and simple formulas for some physical quantities in two quantum chains. A classic result of this type is Onsager, Kaufman and Yang’s formula for the spontaneous magnetization in the Ising model, subsequently generalized to the chiral Potts models. We conjecture that analogous results occur in the XYZ chain when the couplings obey $J_x J_y + J_y J_z + J_x J_z = 0$, and in a related fermion chain with strong interactions and supersymmetry. We find exact formulas for the magnetization and gap in the former, and the staggered density in the latter, by exploiting the fact that certain quantities are independent of finite-size effects.

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(Some figures in this article are in colour only in the electronic version)
site $j$ by a variable $\sigma_j = 0 \ldots N - 1$, the exact result as the number of sites goes to infinity
is
\[ \langle e^{2\pi i r \sigma_j/N} \rangle = (1 - k^2)^{(N-r)/(2N^2)}. \]  
(1)

The lattice parameter $k$ in (1) is not renormalized: it is a coefficient of one of the terms in the corresponding quantum Hamiltonian. Nevertheless, the expression for the order parameters in (1) is exact for any value of $k$, ranging from the critical point $k = 1$ to the completely ordered point $k = 0$. This is unusual even for integrable models, when order parameters are computed they are typically given by elaborate combinations of elliptic theta functions (see [10]).

In this communication we conjecture exact formulas analogous to (1) in two quantum chains with strong interactions: the XYZ chain along a special line of couplings [11–14] and interacting fermions with supersymmetry [15, 16]. The conjectures result from studying series expansions around a trivially solvable limit, the analog of $k = 0$ above. We find that for a system with $L$ sites, the terms in these expansions up to order $L$ are independent of $L$. We refer to such quantities as scale free. We can thus compute them exactly by finding the ground states explicitly for small systems. The analogs of (1) then are obtained by summing the series. Since this yields the correct critical exponents for the model, this provides strong evidence that the conjecture is exact in the $L \to \infty$ limit.

To motivate our study, we note two special properties of the chiral Potts model. One is that along a line in parameter space, it possesses a useful symmetry algebra, known as the Onsager algebra [1, 7], which allows the explicit construction of an infinite sequence of conserved quantities. A second (under-appreciated) property is that in the corresponding field theory in the scaling limit, the coefficient of the Lorentz symmetry-breaking perturbation does not renormalize [17].

Supersymmetric field theories also possess such special properties. Because the Hamiltonian is part of the supersymmetry algebra, supersymmetry does much more than just grouping of states into multiplets. One can often prove the existence of zero-energy ground states by computing the Witten index [18]. Moreover, in some cases there are non-renormalization theorems. For example, in the scaling limit of the models described below, the superpotential does not receive any corrections beyond tree level in perturbation theory [19]. This means that some physical quantities (for example, the gaps of certain kink states) depend simply on the parameters in the Hamiltonian.

This motivates us to study quantum chains whose scaling limits are described by supersymmetric field theories. Our first example is a special case of the well-known XYZ chain[10]. The Hilbert space $(\mathbb{C}^2)^\otimes L$ is a two-state system at each site on the chain, and the Hamiltonian is
\[ H = - \sum_{j=1}^L \left[ J_x \sigma_x^j \sigma_x^{j+1} + J_y \sigma_y^j \sigma_y^{j+1} + J_z \sigma_z^j \sigma_z^{j+1} + E_0 \right], \]  
(2)
where the $\sigma^a$ are the Pauli matrices and $E_0$ is a constant. For now we take periodic boundary conditions, so that $\sigma_{L+1}^a \equiv \sigma_1^a$. When $J_x = J_y$, the Hamiltonian preserves the numbers of up-spins and down-spins individually; elsewhere these numbers are only conserved mod 2. For $L$ odd, all states including the ground state are therefore paired by flipping all the spins. If one of the $J_a$ vanishes, the chain can be mapped onto free fermions by the usual Jordan–Wigner transformation; otherwise, the mapping gives interacting fermions. Whenever $J_x = J_y$ and $|J_z| \leq J_x$ (and values related by permuting the $J_a$), the model is critical and is called the XXZ chain. Along this critical line, a free-boson field theory describes the scaling limit. Near this critical line, it can be described by the sine-Gordon field theory.

The field theory of the XYZ chain is supersymmetric along a particular line in its two-parameter space (see e.g. [20]). Because the chain is integrable [10], it is easy to identify
the supersymmetric critical point in the XXZ chain: it is at $J_z = -|J_x|/2$. The XXZ chain here has many fascinating properties (see e.g. [21]). In fact, long ago Baxter found a simple formula for the exact ground-state energy as $L \to \infty$ along the entire line

$$J_x J_y + J_z J_z + J_x J_z = 0. \quad (3)$$

Namely, for $E_0 = -(J_x + J_y + J_z)$, the ground-state energy along this line goes to zero as $L \to \infty$. Moreover, it was conjectured that the lowest eigenvalue of $H_{\text{XYZ}}$ along this line is exactly zero when $L$ is odd [21], just as in supersymmetric models. This was subsequently proved (for $L$ odd as well as for $L$ even with twisted boundary conditions) at the critical point by showing that the XXZ chain has a hidden supersymmetry relating chains with different numbers of sites [16, 22]. Moreover, there are a host of other fascinating and special results along this line [12–14], all reminiscent of the special results occurring in fermion chains with an explicit supersymmetry [15, 16, 23]. Thus, the XYZ chain along the line (6) indeed should correspond to a supersymmetric field theory in the scaling limit; for this reason we dub this the sXYZ chain.

Our second chain is a staggered version of a fermion chain with a built-in supersymmetry [15, 16]. These models are defined from the supersymmetry operator $Q$ obeying $Q^2 = 0$. The Hamiltonian $H = QQ^\dagger + Q^\dagger Q$ then commutes with $Q$ and $Q^\dagger$. We study the supersymmetric Hamiltonian acting on a Hilbert space spanned by spinless fermions, with the additional restriction that fermions may not be on adjacent sites. The supersymmetry operator in terms of fermion creation operators $c_j^\dagger$ is

$$Q = \sum_j \lambda_j (1 - n_{j-1})(1 - n_{j+1})c_j, \quad (4)$$

where $n_j = c_j^\dagger c_j$. $Q$ squares to zero for any choice of the complex numbers $\lambda_j$, so the Hamiltonian

$$H_{\text{sfF}} = \sum_{j=1}^{3f} \left[ (1 - n_{j-1})(1 - n_{j+1})c_j^\dagger c_j + \text{h.c.} \right]$$

is supersymmetric. The first term allows hopping preserving the restriction, and the second comprises a chemical potential and a next-nearest-neighbor repulsion. When the number of fermions is $f$ and the number of sites is $3f$, for periodic boundary conditions there are two ground states for any values of the $\lambda_j$ [15]. Here we consider the staggering $\lambda_{3j} = \lambda_{3j+1} = 1$ and $\lambda_{3j+2} = z$, and so we label this model ssF (for supersymmetric staggered Fermions).

The Bethe equations for the unstaggered case $z = 1$ and for the critical sXXZ chain are the same up to boundary conditions [16], and so the critical field theories must be the same. Staggering the model perturbs it away from this critical point, and since there is only one Lorentz-invariant supersymmetry-preserving perturbation, its scaling limit should be the same as the supersymmetric field theory describing sXYZ.

For the remainder of this communication we describe some of the remarkable properties of these models. The key to much of our analysis is to expand various quantities around a limit where the model can be solved trivially. An amazing property of these chains is that for certain quantities, the coefficients of the terms in this expansion are scale free.

We parametrize the sXYZ line (3) by

$$J_x = 2s(s - 3), \quad J_y = 2s(s + 3), \quad J_z = 9 - s^2, \quad (6)$$

so that $E_0 = -3(s^2 + 3)$. The critical points are at $s = \pm 1, \infty$, while at the trivially solvable points $s = 0, \pm 3$ only one of the three terms in (2) remains. At $s = 0$, only $J_z \neq 0$, so the ground state $|0\rangle$ has all spins the same. The spontaneous magnetization per site $M_L(s) \equiv \langle 0|\sigma_j^z|0\rangle$ obeys $M_L(0) = 1$ in the sector with an even number of down spins. We
find, by using Maple to compute the exact ground state, that the power-series expansions of the magnetization for odd $L$ are

$$
M_5 = 1 - 4s^2 - 12s^4 + 188s^6 - 844s^8 + 380s^{10} + \cdots \\
M_7 = 1 - 4s^2 - 12s^4 - 52s^6 + 2516s^8 - 18004s^{10} + \cdots \\
M_9 = 1 - 4s^2 - 12s^4 - 52s^6 - 284s^8 + 33516s^{10} + \cdots \\
M_{11} = 1 - 4s^2 - 12s^4 - 52s^6 - 284s^8 - 1764s^{10} + \cdots 
$$

where $s = \theta/3$. The trend is obvious: the order $s^n$ terms in the expansion are independent of $L$ when $n < L$. The magnetization appears to be scale free near $s = 0$. Doing this to $L = 17$ yields what is presumably the exact expansion as $L \to \infty$:

$$
M_L(s) = 1 - 4s^2 - 12s^4 - 52s^6 - 284s^8 - 1764s^{10} - 11820s^{12} - 83220s^{14} - 606780s^{16} + \cdots 
$$

To understand how to sum the series and find a simple formula for $M_\infty(s)$, we examine the expected behavior at the critical point $s = 1$. The dimension of the ‘thermal’ operator that perturbs away from $s = 1$ onto the sXYZ line is $4/3$, while the dimension of the magnetization operator is expected to be $1/3$ [10]. Indeed, the finite-size values at criticality fit nicely to $M_L(s) = 0.95527 L^{-3/5} (1 + O(L^{-2}))$. Thus, as $s \to 1^-$, $M_\infty(s)$ should vanish as $(1 - s)^\beta$ with $\beta = (1/3)/(2 - 4/3) = 1/2$. This square-root singularity suggests looking at the series expansion of $(M_L(s))^{2}$:

$$(M_L(s))^{2} = 1 - 8s^2 - 8s^4 - 8s^6 - 8s^8 - 8s^{10} - 8s^{12} - 8s^{14} - 8s^{16} + O(s^{L+1}).$$

Summing this series yields a conjecture for the exact magnetization in the ordered phase $s < 1$:

$$
M_\infty(s) = 3 \left(\frac{1 - s^2}{9 - s^2}\right)^{1/2}. 
$$

We emphasize that we do not assume anything about the behavior at the critical point $s = 1$; the only role of the scaling argument is to suggest that we square $M$. The fact that the expected critical behavior for the magnetization emerges from the expansion around $s = 0$ is to us a compelling argument that formula (7) is exact.

We plot this function and the finite-size curves in figure 1. Even with the finite-size effects near $s = 1$, it is clear that the finite-$L$ curves are approaching the conjectured curve. A numerical calculation using the iTEBD method gives the same curve to high accuracy [24]. Moreover, with a change of variables, (7) gives the same ‘$q$-series’ obtained by exploiting the integrability of the chain. The corresponding quantity in the eight-vertex model, the spontaneous polarization, is [25, 26]

$$
P_0 = \frac{4\pi}{2\pi - \eta} \left( \frac{\partial q(0, q^{1/2})}{\partial \tilde{\alpha}(0, q^{1/2})} \right)^2 
$$

when written in terms of Jacobi theta functions [27]. The sXYZ line (3) corresponds to setting the crossing parameter $\eta = \pi/3$. Using the Boltzmann weights of the eight-vertex model at this point, we find

$$
s = 3 \left( \frac{\partial q(\pi/3, q^{1/2})}{\partial \tilde{\alpha}(\pi/3, q^{1/2})} \right)^2 
$$

for $0 < s < 1$. Inserting this into (7) yields the same expansion in $q$ as that of (8) to $\sim 500$ terms.
We have found other exact formulas using these methods. Letting \( H_j^s = \sigma_j^x \sigma_{j+1}^x \) for \( s < 1 \)

\[
\langle 0 | H_j^s | 0 \rangle = 1 + 4s^2(-1 + s^2 + 3s^4 + 5s^6 + 7s^8 + \cdots)
\]

\[
= 1 + 12 \frac{s^2(s^2 - 3)}{(s^2 - 9)^2} + O(s^{L+1}).
\]  

(10)

We can find this expectation value for \( s > 1 \) by expanding around \( s = 3 \), where \( J_x = J_z = 0 \).

Letting \( t = (3 - s)/6 \),

\[
\langle 0 | H_j^s | 0 \rangle = \frac{1}{2} \left( 2t + 3t^2 + 4t^3 + 5t^4 + \cdots \right)
\]

\[
= \frac{(s + 9)(3 - s)}{2(3 + s)^2} + O(t^{L+1}).
\]  

(11)

Using the \( q \)-series representation (9) we showed analytically that (10) matches the exact results [28]. The expectation values of \( H_j^x \) and \( H_j^y \) can be found from these by using the duality symmetries \( s \rightarrow (3 - s)/(s + 1) \) and \( s \rightarrow -s \), or by using the Hellmann–Feynman theorem \( \langle 0 | dH_{XYZ}/ds | 0 \rangle = 0 \).

Not only ground-state properties are scale free but the gap is as well and obeys an elementary formula. To define the gap, we exploit the fact that there is a spontaneously broken \( Z_2 \) symmetry away from the critical points. It is thus natural to think of the gapped excited states as kinks separating regions of the two ground states. This picture is supported by the computation of the exact scattering matrix for these kinks in the supersymmetric field theory [20]. For an odd number of sites and periodic boundary conditions, we expect the lowest-energy excited states to be two-kink states. Since the kinks interact, the energy is less than twice the kink gap. Thus, to define the gap to the one-kink state, we consider an \( even \) number of sites with twisted boundary conditions (a spin-flip defect): \( \sigma_{n+1}^z = -\sigma_n^z \), \( \sigma_{n+1}^y = -\sigma_n^y \) and \( \sigma_{n+1}^x = +\sigma_n^x \). Near \( s = 0 \), the interactions away from the boundary favor aligning the spins, but the twist forces the energy to be order \( J_z \).

The result for the gap is more transparent when we rescale the Hamiltonian \( H \rightarrow H/s^2 \) and consider the region between the trivially solvable point \( s = 3 \) and the critical point at \( s \rightarrow \infty \); the gap in other regions is obtained by exploiting duality. We found the exact one-kink energy \( \Delta \) for sizes up to \( L = 10 \). Expanding this in a power series around \( s = 3 \) in
terms of \( v = 1 - 3/s \), we find
\[
\Delta_L = 4 - 6v + 3v^2/2 + v^3/4 + 3v^4/32 + \cdots
= 4 \left( \frac{3}{s} \right)^{3/2} + O(v^{1/2}).
\] (12)

Thus at the critical point \( s \to \infty \), the gap vanishes with the exponent \( v = 3/2 \). This is exactly what one expects with dimension-4/3 thermal operator: \( v = 1/(2 - 4/3) = 3/2 \).

We now turn to the supersymmetric staggered fermion model with Hamiltonian (5) and show that not only does it possess scale-free quantities similar to those of the sXYZ chain but that the models are deeply related on the lattice, not just in their scaling limits. For \( f \) fermions on \( 3f \) sites, \( H_{sF} \) has two zero-energy ground states like \( H_{sXYZ} \). Here, however, the two ground states are not related by symmetry: because the fermions cannot occupy adjacent sites, there is no analog of spin-flip symmetry. To define basis vectors for the two-dimensional space of zero-energy states unambiguously, we exploit the parity symmetry \( j \to 3f + 1 - j \). One ground state, denoted \(|+\rangle_z \), is even under parity, while the other ground state \(|-\rangle_z \) is odd. These two ground states are quite different from each other, as is easy to see by studying them in the solvable limits.

We find exact formulas for the staggered fermion densities \( D^\pm(z) = \langle \pm | c_{j+1}^\dagger c_{j-1} | \pm \rangle_z \). These have been studied at the critical point \( z = 1 \), using numerics [23] and using conformal field theory [29], and we extend these results to all \( z \). In the solvable limits, we have \( D^+(\infty) = D^-(\infty) = D^+(0) = 0 \) and \( D^-(0) = 1 \). Moreover, at the critical point \( z = 1 \), the full translation symmetry of the model is restored. This requires that \( D^+(1) + D^-(1) = 2/3 \). Thus we expect that \( D^+ = D^- \) behaves like the magnetization in the sXYZ chain, vanishing as \( f \to \infty \) when \( z \geq 1 \), but non-zero for \( z < 1 \). By finding the exact ground state in sizes up to \( f = 8 \) (24 sites), we obtain for \( z \) small
\[
D^+ + D^- = 1 - 3\tilde{z}^2 + 3\tilde{z}^4 - 3\tilde{z}^6 + 3\tilde{z}^8 - \cdots
= \frac{8 - 2\tilde{z}^2}{8 + \tilde{z}^2} + O(z^{1/2}).
\] (13)
\[
D^+ - D^- = 1 - 2\tilde{z}^2 - 3\tilde{z}^4 + 29\tilde{z}^6 - 131\tilde{z}^8 - \cdots
= \frac{8\sqrt{7} - \tilde{z}^2}{8 + \tilde{z}^2} + O(z^{1/2}).
\] (14)

where \( \tilde{z} = z/\sqrt{8} \). We see the same square-root singularity in \( D^+ - D^- \) that we did for the magnetization in sXYZ. The series expansion around \( z = \infty \) gives
\[
D^+ + D^- = \frac{2}{z^2} - \frac{6}{z^4} + \frac{26}{z^6} - \frac{134}{z^8} + \frac{762}{z^{10}} - \frac{4614}{z^{12}} + \cdots
= \frac{4}{z^2 + z\sqrt{8} + z^2 + 2} + O(z^{-4/3}).
\] (15)

The finite-size curves for \( D^+ + D^- \) are almost indistinguishable from the asymptotic form, because of the exact result at \( z = 1 \) and the scale-free behavior in the small- and large-\( z \) limits. The curves for \( D^+ - D^- \) are plotted in figure 2.

Field-theory dualities need not be exact in the corresponding lattice models or can be very subtle (e.g. the Kramers–Wannier duality of the Ising model). Thus, even though the
sXYZ chain has the duality symmetry \( s \rightarrow (3 - s)/(s + 1) \), the corresponding duality is not obvious in the ssF chain. Nevertheless, we have non-trivial evidence that there is such a duality exchanging the \( |z| > 1 \) and \( |z| < 1 \) phases. This becomes apparent when we simplify (15) by defining the new coupling \( S = 3z/\sqrt{z^2 + 8} \), so that \( D^+ + D^- = 2(3 - S)/(3S + 3) \) asymptotically for \( z > 1 \). The \( z = 1 \) critical point is at \( S = 1 \), while the solvable points \( z = 0 \) and \( z = \infty \) correspond to \( S = 0 \) and \( S = 3 \), respectively, the same as the value of \( s \) in the sXYZ chain. We find that

\[
D^+(S)D^-(S) = D^+(\hat{S})D^-(\hat{S})
\]

for \( \hat{S} = (3 - S)/(S + 1) \). This relation holds for all finite sizes up to \( 3f = 24 \) sites, and of course for the asymptotic formulas as well. It thus seems very likely that this is a general symmetry of the ssF chain, but we have not yet found the corresponding symmetry of the Hamiltonian.

The relation between the sXYZ and ssF chains goes even deeper. In a remarkable series of papers [13], Bazhanov and Mangazeev showed that (at least for small systems) the ground states themselves are related to the tau functions of the Hamiltonian hierarchy of the Painlevé VI nonlinear differential equation. They find a recursion relation for the coefficient of the state with all spins down in the wavefunction, normalized so that it is a polynomial in \( s \). This same polynomial appears in the ground state in our ssF chain! It appears (up to a convention-dependent overall power of \( S \)) for example as the coefficient in \( |+\rangle \), of the state \( |2\rangle \) defined above, when \( z \) is rewritten in terms of \( S \). Moreover, the normalizations of the ground states are related to the same polynomials, just as in [13]. Thus, the ssF ground states can be related in the same fashion to Painlevé VI.

We have presented conjectures for exact results in two interacting chains. These include simple formulas for the spontaneous magnetization and the gap in the XYZ chain when the scaling limit is a supersymmetric field theory. We believe that the evidence for these conjectures is convincing. Moreover, these chains quite obviously have a great deal of symmetry structure left to be uncovered. In particular, all the evidence—the scale free property, the important role of supersymmetry and the precise relations between the ground states of the two chains—makes it seem likely to us that there is an infinite-dimensional symmetry in both models similar to the Onsager algebra [1]. Each model will then correspond to a different presentation of this algebra.
Note added in proof. We have succeeded in proving equation (7) for the sXYZ magnetization from equation (8) by deriving theta-function identities applicable at \( \eta = \pi/3 \).

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References

[1] Onsager L 1944 Phys. Rev. 65 117
[2] Kaufman B 1949 Phys. Rev. 76 1232
[3] Kaufman B and Onsager L unpublished (the result was announced at several conferences)

Onsager L 1949 Nuovo Cimento Suppl. 6 261 as reproduced in 1996 The Collected Works of Lars Onsager (with Commentary) (Singapore: World Scientific)
[4] Yang C N 1952 Phys. Rev. 85 585
[5] McCoy B and Wu T T 1973 The Two-Dimensional Ising Model (Cambridge, MA: Harvard University Press)
[6] Howes S, Kadanoff L P and den Nijs M 1983 Nucl. Phys. B 215 169
[7] von Gehlen G and Rittenberg V 1985 Nucl. Phys. B 257 351
[8] Albertini G, McCoy B M, Perk J H H and Tang S 1989 Nucl. Phys. B 314 741
[9] Baxter R J 2005 Phys. Rev. Lett. 94 130602
[10] Baxter R J 2010 J. Phys. A: Math. Theor. 43 145002
[11] Baxter R J 1982 Exactly Solved Models in Statistical Mechanics (London: Academic)
[12] Baxter R J 1972 Ann. Phys. 70 323
[13] Bazhanov V V and Mangazeev V V 2005 J. Phys. A: Math. Gen. 38 L145

Bazhanov V V and Mangazeev V V 2006 J. Phys. A: Math. Gen. 39 12235

Bazhanov V V and Mangazeev V V 2010 J. Phys. A: Math. Theor. 43 085206
[14] Razumov A V and Stroganov Yu G 2009 arXiv:0911.5030
[15] Fendley P, Schoutens K and de Boer J 2003 Phys. Rev. Lett. 90 120402
[16] Fendley P, Nienhuis B and Schoutens K 2003 J. Phys. A: Math. Gen. 36 12399
[17] Cardy J L 1993 Nucl. Phys. B 389 577
[18] Witten E 1982 Nucl. Phys. B 202 253
[19] Martinec E J 1990 Physics and Mathematics of Strings (Singapore: World Scientific)

Vafa C and Warner N P 1989 Phys. Lett. B 218 51
[20] Fendley P and Intriligator K 1992 Nucl. Phys. B 372 533
[21] Stroganov Yu 2001 J. Phys. A: Math. Gen. 34 L179
[22] Yang X and Fendley P 2004 J. Phys. A: Math. Gen. 37 8937
[23] Beccaria M and De Angelis G F 2005 Phys. Rev. Lett. 94 100401
[24] Pollmann F private communication
[25] Baxter R J and Kelland S B 1974 J. Phys. C: Solid State Phys. 7 L403
[26] Jimbo M, Miwa T and Nakayashiki A 1993 J. Phys. A: Math. Gen. 26 2199

Lashkheveich M and Pugai Y 1998 Nucl. Phys. B 516 623
[27] Whittaker E T and Watson G N 1927 A Course of Modern Analysis (Cambridge: Cambridge University Press)
[28] Boos H, Jimbo M, Miwa T, Smirnov F and Takeyama Y 2005 J. Phys. A: Math. Gen. 38 7629
[29] Huijse L 2010 University of Amsterdam Thesis