

Critical theory of quantum spin chains

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The relation between quantum spin chains and conformal field theories is reexamined. Using a generalized Hubbard model representation it is argued that the critical theory for generic half-odd-integer spin antiferromagnets is the Wess-Zumino-Witten model (WZW model) with topological coupling, $k=1$, whereas generic integer spin antiferromagnets have an energy gap. The higher- k WZW models (which describe integrable higher spin models) are multicritical points in the space of all spin Hamiltonians. The $k=1$ WZW model represents a stable fixed point for many theories including WZW models of arbitrary odd k with relevant operators added, generalized Hubbard or Thirring models with an odd number of colors and the $O(3)$ σ model at topological angle $\theta=\pi$.

Quantum spin chains were studied¹ using non-Abelian bosonization² in a recent paper. It was suggested that, at least in some cases, the critical theory for a spin- s antiferromagnet is the Wess-Zumino-Witten nonlinear σ model (WZW model) with topological coupling $k=2s$. In general, except in the case $k=1$, there are relevant operators in these models respecting all obvious symmetries of the spin systems. One might expect that if these operators were present they would produce a gap. Given the independent arguments that a gap exists for integer, but not half-odd integer s , it was speculated that these operators were generated in the former but not the latter case. It was difficult to resolve this issue, in part because of uncertainties in the non-Abelian bosonization procedure for $k>1$. In two later papers, it was shown that the low-temperature susceptibility³ and specific heat⁴ are determined by k and the conformal anomaly parameter $c=3k/(2+k)$, respectively. This allowed for a demonstration that the integrable Hamiltonians⁵ of arbitrary spin were indeed in the $k=2s$ universality class.

In this paper we wish to reexamine these issues. We will obtain spin- s antiferromagnets from the infinite (Hund's rule) coupling limit of a generalized Hubbard model with $2s$ orbitals. An approximate mapping onto the $k=2s$ WZW model using non-Abelian bosonization suggests that relevant operators are generally induced for all $k>1$. By adjusting enough parameters in the spin Hamiltonian, the coefficients of all relevant operators can presumably be made to vanish. The number of such relevant operators is the largest integer j such that $j \leq k/2$ and $j(j+1) < 2+k$. It thus appears that the integrable Hamiltonians correspond to such special multicritical points.

The effect of relevant operators is then considered in more detail. It is argued that they tend generically to produce a gap for k even, but to produce crossover to the $k=1$ fixed point for k odd. Passing to the large k limit a semiclassical argument indicates that the relevant

operators lead to a low-energy theory which is the $O(3)$ σ model with Π_2 topological term equal to $k\pi$. This is in accord with previous arguments⁶ that this is the low-energy theory for a large- s spin chain, with $\theta=2\pi s$ and indicates that the critical theory for the $O(3)$ σ model at $\theta=\pi$ is the $k=1$ WZW model (not the $k=\infty$ WZW model as the previous discussion¹ suggested). Indeed the $k=1$ WZW model represents a stable fixed point for many $SU(2)$ invariant systems due to a type of topological stability.

In Ref. 3 the spin-wave velocity times zero-temperature susceptibility of $(\text{CH}_3)_4\text{NMnCl}_3$ (TMMC), a highly one-dimensional antiferromagnetic, was shown to be fairly close to the value corresponding to $k=5$ ($=2s$). However, as was also pointed out, the $k=5$ value happens to be very close to the classical value for this quantity and, since $s=\frac{5}{2}$ is fairly large, one should expect the classical approximation to be quite good down to low temperatures where quantum effects dominate. The temperature at which quantum effects become important is exponentially small for large s : $O(e^{-\pi s})$. We now believe that this "quantum temperature" is below the Néel temperature for TMMC (0.85 K) where three-dimensional effects become dominant. Extracting one-dimensional critical exponents from these systems is further complicated by the fact that even small anisotropies produce large effects at low T and large s . Thus we are rather pessimistic about the prospects for experimental observation of the one-dimensional critical behavior described in this paper, for $s \geq \frac{3}{2}$. There is perhaps some chance in a very one-dimensional and very isotropic $s=\frac{3}{2}$ antiferromagnet. The numerical results for $s=\frac{3}{2}$ may be useful in this regard.⁷

We begin with the standard spin- s antiferromagnetic Heisenberg model:

$$H = J \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1}, \quad \mathbf{S}_n^2 = s(s+1). \quad (1)$$

We find it convenient to use a generalized Hubbard model representation for the spin chain. The relation between the ordinary Hubbard model and the $s = \frac{1}{2}$ antiferromagnet was used, for example, in Ref. 8. The model actually mimics the way spins are produced from electrons in real crystals. The best higher spin antiferromagnets [such as $(\text{CH}_3)_4\text{NMnCl}_3$] with $s = \frac{5}{2}$ have transition metals as the magnetic ions, with half-filled outer d shells (such as Mn^{2+}). A strong Hund's-rule coupling between the five electrons in the d shell of each ion makes the spins line up, forming an $s = \frac{5}{2}$ spin variable. The weaker exchange forces between electrons of *neighboring* ions then produce the antiferromagnetic interaction between the spins. In our model we will introduce $2s$ identical half-filled orbitals per lattice site to obtain spin s . The Hamiltonian contains a nearest-neighbor hopping term and a Hund's rule coupling which is taken to infinity. We will refer to the orbital index, $i = 1, 2, \dots, n_c$ as the *color*. The numbers of colors $n_c = 2s$. $\psi_{i\alpha n}$ annihilates an electron of color i , spin α (equal $\pm \frac{1}{2}$) at site n . Repeated spin or color indices are implicitly summed over. Thus the spin variables are written as

$$\mathbf{S}_n = \sum_i \mathbf{S}_{in} = \frac{1}{2} \psi_n^{\dagger i\alpha} \boldsymbol{\sigma}^\alpha \psi_{i\beta n}, \quad (2)$$

where \mathbf{S}_{in} is the spin of the color i electron and the σ^α 's are Pauli matrices. The Hund's-rule (HR) coupling is

$$H_{\text{HR}} = -U \sum_n \mathbf{S}_n^2.$$

Using the identity

$$\sigma^\alpha_\beta \cdot \sigma^\gamma_\epsilon = 2\delta^\alpha_\epsilon \delta^\gamma_\beta - \delta^\alpha_\beta \delta^\gamma_\epsilon,$$

this can be written

$$H_{\text{HR}} = (U/4) \sum_n [2(\psi_n^{\dagger i\alpha} \psi_{j\alpha n} - \delta^i_j)(\psi_n^{\dagger j\beta} \psi_{i\beta n} - \delta^j_i) + (\psi_n^{\dagger i\alpha} \psi_{i\alpha n} - n_c)^2].$$

Here we have dropped constants and terms proportional to the (conserved) total electron number. It can be seen that the ground states of H_{HR} are all states with n_c electrons per site in a color singlet state (i.e., antisymmetric with respect to color). Such states have spin $s = n_c/2$. The hopping term is

$$H_0 = -\frac{1}{2} \sqrt{n_c} J U \sum_n [\psi_n^{\dagger i\alpha} \psi_{i\alpha n} + 1 + \text{H.c.}]$$

where H.c. stands for Hermitian conjugate. Note that the full Hamiltonian is invariant under an $\text{SU}(n_c)$ color symmetry and that the Hund's-rule coupling favors local color singlet states. This is very reminiscent of quantum chromodynamics where the Hund's-rule coupling results effectively from exchange of gluons (however, this leads to a long-range force, not a local one). The low-energy states of the Hubbard model correspond to baryons (color singlets formed antisymmetrically out of quarks) with residual spin interactions. In the limit $U \rightarrow \infty$, the Hamiltonian, projected onto the low-energy states, becomes simply the Heisenberg Hamiltonian. This can be

seen by considering perturbation theory in the hopping term. Only second-order perturbation theory survives as $U \rightarrow \infty$. The intermediate state has $s = (n_c \pm 1)/2$ on two sites and hence excitation energy, $\Delta E = U/2$. This representation can be generalized to any dimension.

We will extract the critical theory for the antiferromagnetic *chain* out of this representation by considering first the case of small U ($U \ll J$). The motivation is the same as in the more familiar case of the ordinary Hubbard model.⁸ We will search for a possible gapless low-energy sector of the theory at small U . The remaining states will have a gap that grows with U [being of order $\exp(-\text{const} \times \sqrt{J/U})$ at small U]. The gapless sector is decoupled from the other states. Therefore the effect of taking $U \rightarrow \infty$ is simply to give these other states infinite energy.

Thus we begin by ignoring entirely the Hund's-rule interaction term in the Hamiltonian. The hopping term gives a dispersion relation

$$E = (v/a) \cos ak$$

where $v \equiv 2\sqrt{JU}a$ is the Fermi velocity and a is the lattice spacing. The Fermi "surface" is at $k = \pm\pi/2a$, for a half-filled band. The low-energy states are electrons just above and holes just below, the Fermi surface. Thus we are only concerned with Fourier modes of the electron annihilation operators $\psi_{i\alpha n}$ with $k \approx \pm\pi/2a$. We write

$$a^{-1/2} \psi_{i\alpha n} \approx e^{i\pi n \alpha/2} \psi_{L i \alpha}(an) + e^{-i\pi n \alpha/2} \psi_{R i \alpha}(an), \quad (3)$$

where $\psi_{L,R}$ are slowly varying on the scale of a lattice spacing. ψ_L annihilates electrons and creates holes with $k \approx -\pi/2a$. We refer to these as left-moving electrons and holes. ψ_R annihilates right-moving electrons and creates right-moving holes. In a continuum approximation, suitable for studying the low-energy sector, we linearize the dispersion relation near the Fermi surface. This leads to the continuum Hamiltonian

$$H = iv \int dx [\psi_L^{\dagger i\alpha} (d/dx) \psi_{L i \alpha} - \psi_R^{\dagger i\alpha} (d/dx) \psi_{R i \alpha}].$$

This is the Hamiltonian for massless relativistic Dirac fermions (with color index, i , and spin or flavor index α). v plays the role of the velocity of "light." Henceforth we shall generally set it equal to one. The corresponding Lagrangian density is

$$\mathcal{L} = i(\psi_L^{\dagger i\alpha} \partial_- \psi_{L i \alpha} + \psi_R^{\dagger i\alpha} \partial_+ \psi_{R i \alpha}), \quad (4)$$

where we have introduced "light-cone" coordinates

$$x_\pm \equiv (x_0 \pm x_1)/2, \quad \partial_\pm \equiv \partial_0 \pm \partial_1 (x_0 = t, x_1 = -x^1 = -x).$$

\mathcal{L} is invariant under Lorentz transformations

$$\partial_\pm \rightarrow \partial_\pm e^{\pm\theta}, \quad \psi_{L,R} \rightarrow \psi_{L,R} e^{\pm\theta/2}.$$

Note that, by the equations of motion, $\psi_{R,L i \alpha}$ is a function only of $x_{+,-}$, respectively. We will sometimes consider the light-cone components of the energy-momentum tensor

$$T_{L,R} \equiv (\mathcal{H} \pm \mathcal{P})/2 \equiv i \psi_{L,R}^{\dagger i\alpha} \partial_\pm \psi_{L,R i \alpha},$$

where \mathcal{H} and \mathcal{P} are the Hamiltonian and momentum

densities. $T_{L,R}$ generate translations along the light cone. We will be much concerned with the symmetries and conserved currents of this free fermion theory. All internal symmetries are *chiral*; that is to say we can perform the symmetry operation on the left or right fermions separately. Operating on the left fermions we have a U(1) charge symmetry,

$$\psi_{Li\alpha} \rightarrow e^{i\theta} \psi_{Li\alpha},$$

an SU(2) spin symmetry,

$$\psi_{Li\alpha} \rightarrow g_\alpha^\beta \psi_{Li\beta},$$

and an SU(n_c) color symmetry,

$$\psi_{Li\alpha} \rightarrow h_i^j \psi_{Lj\alpha}.$$

Here, g_α^β and h_i^j are SU(2) and SU(n_c) matrices. Likewise we may make *independent* transformations on the ψ_R 's. The charge, spin, and color of the left- and right-moving fermions are separately conserved. Corresponding to these symmetries we have conserved currents. Introducing the generators of SU(n_c), $(T^A)_i^j$ ($A=1,2,3, \dots, n_c^2-1$; $\text{tr} T^A T^B = \frac{1}{2} \delta^{AB}$; summation of repeated A indices will be implied) the light-cone components of the currents can be written as

$$J_{L,R} \equiv : \psi_{L,R}^{\dagger i\alpha} \psi_{L,R i\alpha} :,$$

$$\mathbf{J}_{L,R} \equiv \psi_{L,R}^{\dagger i\alpha} (\frac{1}{2}) \sigma_\alpha^\beta \psi_{L,R i\beta},$$

$$J_{L,R}^A \equiv \psi_{L,R}^{\dagger i\alpha} (T^A)_i^j \psi_{L,R j\alpha}.$$

Here the double dots denote normal ordering. The energy-momentum tensor can be written in a form quadratic in currents:¹

$$T_L = (\pi/2n_c) v \mathbf{J}_L \cdot \mathbf{J}_L + [2\pi/(n_c+2)] v \mathbf{J}_L \cdot \mathbf{J}_L + [2\pi/(n_c+2)] v J_L^A J_L^A \quad (5)$$

(and similarly for T_R). Here we have reinstated the ve-

locity of light v .

We now consider the effect of a small Hund's rule coupling $U \ll J$. We will focus on its effect on the low-energy, relativistic sector of the Hilbert Space. Writing the Hund's rule couplings in terms of $\psi_{L,R}$ we obtain terms with four powers of ψ_L (or four powers of ψ_R) and also terms with two ψ_L 's and two ψ_R 's. Only four Fermi terms with no derivatives will be retained. The higher-derivative terms are irrelevant at the free fermion fixed point and also at the nontrivial fixed points which we will encounter later. The completely left-moving (or completely right-moving) terms can be written quadratically in the currents and thus simply renormalize the speed of light in (5). This renormalization is different for the terms in (5) involving charge, spin, and color currents:

$$\delta v_{\text{spin}} = -(n_c+2)U/2\pi,$$

$$\delta v_{\text{charge}} = \delta v_{\text{color}} = 0.$$

A theory with three different velocity of lights could not, of course, be Lorentz invariant. However, as we shall see, only the spin part of T_L will be retained in the low-energy theory so only the spin velocity parameter will be relevant.

The left-right terms correspond to Lorentz-invariant interaction terms in the Lagrangian of (4) (the same terms as in the Hamiltonian, but with a change of sign). Thus they can be treated using field-theoretic methods. There are actually six different Lorentz-invariant interactions permitted by the symmetries of the Hubbard model. We see from the definition of the continuum Fermi fields, (3), that the single charge spin and color symmetries of the Hubbard model correspond to the diagonal subgroup of the chiral symmetries of the free field theory, under which left and right fermions transform the same way. The six interactions permitted by these diagonal symmetries are

$$\begin{aligned} \mathcal{L}_{\text{int}} = & \lambda_1 \mathbf{J}_L \cdot \mathbf{J}_R + \lambda_2 \mathbf{J}_L \cdot \mathbf{J}_R + \lambda_3 J_L^A J_R^A + \lambda_4 (\psi_L^{\dagger i\alpha} (T^A)_i^j \sigma_\alpha^\beta \psi_{Lj\beta}) (\psi_R^{\dagger k\gamma} (T^A)_k^l \sigma_\gamma^\delta \psi_{Rl\delta}) \\ & + \lambda_5 [(\epsilon_{\alpha\beta} \psi_L^{\dagger i\alpha} \psi_L^{\dagger j\beta}) (\psi_{Ri\gamma} \psi_{Rj\delta} \epsilon^{\gamma\delta}) + \text{H.c.}] + \lambda_6 (\psi_L^{\dagger i\alpha} \psi_L^{\dagger j\beta} \psi_{Ri\alpha} \psi_{Rj\beta}) + \text{H.c.} \end{aligned} \quad (6)$$

Here $\epsilon_{\alpha\beta}$ is the antisymmetric tensor ($\epsilon_{12}=1$) and the curly brackets indicate symmetrization of the spin indices. Due to Fermi statistics the fifth term which is antisymmetric in (left and right) spin indices is symmetric in color indices and conversely for the sixth term. These coupling constants have the values (with $v=1$)

$$\lambda_1 = -3aU/4n_c, \quad \lambda_2 = (2+1/n_c)aU, \quad \lambda_3 = -3aU/2, \quad \lambda_4 = 8aU, \quad \lambda_5 = 3aU/8, \quad \lambda_6 = -aU/4. \quad (7)$$

We will be interested in more general Hamiltonians than the basic Heisenberg model of (1). In particular we may wish to allow arbitrary polynomial nearest-neighbor interactions as well as second (and possibly higher) nearest-neighbor interactions:

$$H = \sum_n [P_1(\mathbf{S}_n \cdot \mathbf{S}_{n+1}) + P_2(\mathbf{S}_n \cdot \mathbf{S}_{n+2}) + \dots].$$

The arbitrary functions P_1, P_2 can be assumed without loss of generality to be polynomials of degree $2s$. These can be incorporated into the Hubbard model formulation by simply making the replacement (2) for the spins in all terms beyond the basic Heisenberg Hamiltonian. Taking all these additional interactions to be small we may treat them perturbatively. They have the effect of renormalizing the speed(s) of light and the coupling con-

stants, λ_1 to λ_6 . Operators of higher order than quartic in the fermion fields are also generated. However, these are irrelevant at the (unstable) free fermion fixed point. We *will* effectively consider them later after locating the nontrivial fixed points. For example, a bilinear nearest-neighbor exchange term

$$\delta H = J_b \sum (\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2$$

gives, in the continuum limit,

$$\delta H = (J_b) \{ [(\mathbf{J}_L + \mathbf{J}_R)^2 - (\psi_L^{\dagger\alpha} \sigma_\alpha^\beta \psi_{R\beta} + \text{H.c.})^2]^2 + [(\mathbf{J}_L - \mathbf{J}_R) \cdot (\psi_L^{\dagger\alpha} \sigma_\alpha^\beta \psi_{R\beta} + \text{H.c.})]^2 \} .$$

Wick, contracting two pairs of fermion fields, gives operators quartic in the fermion fields. (Using the lattice propagator this calculation is ultraviolet finite.) Thus in general we should consider the six coupling constants, λ_i , to be arbitrary parameters.

We wish to discuss first the case $s = \frac{1}{2}$ which is much simpler than the others. This is so because there are no color degrees of freedom in this case and consequently the third, fourth, and sixth terms in (6) vanish. The fifth term is invariant under *chiral* SU(2); this implies that it does not couple to the SU(2) currents but only the U(1) currents. Thus the renormalization-group equation for λ_2 decouples from those for λ_1 and λ_5 :

$$d\lambda_1/d \ln L = -(16/\pi)\lambda_5^2 ,$$

$$d\lambda_5/d \ln L = -(4/\pi)\lambda_1\lambda_5 ,$$

$$d\lambda_2/d \ln L = -(1/\pi)\lambda_2^2 .$$

This decoupling is actually an exact feature of the field theory (true to all orders in perturbation theory). A nice way of seeing this is to bosonize. Abelian or non-Abelian bosonization work equally well in this case, but we choose the non-Abelian version because it keeps the SU(2) symmetry manifest and because it is related to the discussion of higher s , given below. Thus the charge degrees of freedom are represented by an ordinary massless free boson field, φ , but the spin degrees of freedom by an SU(2) matrix, $g^{\alpha\beta}$:

$$\mathcal{L}(\varphi) = \frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi ,$$

$$S_{\text{WZW}}(g) = (1/8\pi) \int d^2x \text{tr} \partial_\mu g^\dagger \partial^\mu g + (1/12\pi) \int d^3x \epsilon^{\mu\nu\lambda} \text{tr} g^\dagger \partial_\mu g g^\dagger \partial_\nu g g^\dagger \partial_\lambda g .$$

The second (Wess-Zumino) term is defined by extending the two-dimensional space (or space-time) to a three-dimensional half-space ($x_3 < 0$) and $g(x_\mu)$ is an arbitrary extrapolation of the function defined on the two-dimensional space (at $x_3 = 0$) which approaches 1 at $x_3 \rightarrow -\infty$. The boundary value determines the Wess-Zumino term up to a term of the form $2\pi n$ (or $2\pi i n$ in Euclidean space) where n is an integer. Thus the path integral is well defined if the coefficient in front of this term is an integer. The coefficient of the first term is then fixed by the condition of chiral symmetry or equivalently by the fixed point of the renormalization group. The currents are written as

$$J_L = (1/\sqrt{4\pi}) \partial_+ \varphi , \quad J_R = -(1/\sqrt{4\pi}) \partial_- \varphi ,$$

$$J_L = -(i/4\pi) \text{tr} \partial_+ g g^\dagger \sigma , \quad J_R = (i/4\pi) \text{tr} g^\dagger \partial_- g \sigma ,$$

and the left-right fermion product as

$$\psi_L^{\dagger\alpha} \psi_{R\beta} \propto g_\beta^\alpha \exp(i\sqrt{2\pi}\varphi) .$$

The fifth interaction term in (6) is independent of g as expected because it only involves the determinant of g which is one. Thus the Lagrangian decouples into separate pieces involving φ and g only:

$$\mathcal{L}(\varphi) = \frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi (1 - \lambda_1/4\pi) + \text{const} \times \lambda_5 \cos \sqrt{8\pi} \varphi ,$$

$$S(g) = S_{\text{WZW}}(g) + \lambda_2 \int d^2x \mathbf{J}_L \cdot \mathbf{J}_R .$$

The renormalization-group equations can be derived in the bosonized version of the theory. Those for φ are very well known. They describe the Kosterlitz-Thouless⁹ transition. For λ_1 negative, as found in (7), the couplings flow to large values and a mass gap appears in the charge sector with

$$m \propto \exp(-\text{const} \times \sqrt{J/U}) .$$

We also anticipate that the symmetry under translation of φ by the period of the cosine will be spontaneously broken. On the other hand, provided that λ_2 is initially positive as found in (7), it renormalizes to zero

$$\lambda_2(L) \rightarrow 1/\pi \ln L .$$

Thus we tentatively conclude that the critical theory for the $s = \frac{1}{2}$ chain is the $k = 1$ WZW model. We should check this conclusion by considering whether there are any relevant operators at this fixed point which could be generated. The only relevant operators allowed by the diagonal SU(2) symmetry are the λ_2 term above and $\text{tr} g$.^{10,11} However, the latter term is odd under the symmetry $g \rightarrow -g$. This symmetry arises in the continuum limit from symmetry under translation by one site in the spin chain, as can be seen from the continuum representation of the spin operators:

$$a^{-1} \mathbf{S}_n \approx (\mathbf{J}_L + \mathbf{J}_R) + \frac{1}{2} (-1)^n (\psi_L^{\dagger\alpha} \sigma_\alpha^\beta \psi_{R\beta} + \text{H.c.}) .$$

Bosonizing the second term and replacing the charge boson by its vacuum expectation value (i.e., integrating it out, since it is massive) we find

$$a^{-1} \mathbf{S}_n \approx (\mathbf{J}_L + \mathbf{J}_R) + i(-1)^n \text{const} \times \text{tr} g \sigma .$$

Thus we see that the symmetry under translation by one site corresponds to changing the sign of g . Therefore, if the Hamiltonian is invariant under this translation, no relevant operators are permitted and the effective Hamiltonian *does* flow to the fixed point, at least for sufficiently small initial couplings. Only terms which break this symmetry or the SU(2) symmetry, such as alternating or nonisotropic exchange or staggered magnetic field, lead to relevant operators.

We now turn to the higher s case. The renormalization group equations now have many more terms since all six couplings are present. Furthermore, the fourth

and sixth operators are nonsinglets under all three chiral groups so that there is no separation of the theory into sectors in general. Let us first consider the case where λ_4 and λ_6 are zero. (This could presumably be achieved by adjusting two parameters in the spin chain Hamiltonian such as biquadratic and second nearest-neighbor couplings.) In this case the fifth term couples together the charge and color degrees of freedom but is a chiral *spin* singlet. Thus the renormalization-group equation for λ_2 separates from that for the other three couplings. Again λ_2 flows to zero assuming it is initially positive, whereas the other three couplings flow to large values. This suggests the existence of a massless decoupled spin sector as for $s = \frac{1}{2}$. But what is the critical theory in this case?

To answer this question let us review a few features of the free fermion theory first.¹ The structure of the energy-momentum tensor in (5) suggests that the theory can be separated into charge, spin, and color sectors. Let us consider the commutation relations obeyed by the currents. We find¹ that the SU(2) currents obey the Kac-Moody algebra with central charge $k = n_c$. This is the algebra obeyed by the currents in the WZW model with topological coupling constant k multiplying the second term in S_{WZW} , and hence also the first term, in order for S to be chirally invariant. Furthermore, this model has an energy-momentum tensor quadratic in currents, as in (5). Indeed this WZW model represents the minimal conformal theory for a given value of k , in the following sense. Given any conformally invariant theory with SU(2) currents obeying the Kac-Moody algebra with central charge k , we may define an energy-momentum tensor quadratic in currents, as in (5). This is not necessarily the full energy-momentum tensor of the theory, but it at least correctly generates space-time translations of the currents themselves (this follows from the current commutation relations). It thus follows that the full energy-momentum tensor can be written as the current part plus an additional part which commutes with all the currents:

$$T_L = T_L^1 + T_L^2, \quad (8)$$

where T_L^1 is the term quadratic in currents and

$$[T_L^2, T_L^1] = [T_L^2, \mathbf{J}_L] = 0.$$

Therefore the conformal anomaly parameter, c , will be the sum of that for T_L^1 [which is $3k/(2+k)$] and that for T_L^2 . Thus the smallest possible value of c (and hence the fewest massless particles) arises when $T_L^2 = 0$. Generally speaking we do not expect accidental massless particles apart from those required by some general principle, like chiral symmetry, so we would expect that the generic critical theory for a conformal system with some specified Kac-Moody algebra would be the corresponding WZW model. Examples of nonminimal models can easily be constructed by adding additional decoupled massless fields which are SU(2) invariant. In this case all operators are simply products of operators in the WZW theory and operators in the decoupled theory. Less trivial cases may also exist. One such example is the

free fermion theory itself. Its energy-momentum tensor (5) takes the general form of (8). However, it is not possible to write $\psi_L^{\dagger\alpha}\psi_{Rj\beta}$ as a product of local operators in the SU(2) WZW theory and in a decoupled theory [the relevant one being a free boson, φ , and an SU(n_c) WZW field, h_j^i , with $k=2$]. Whether some sort of non-local representation, perhaps involving twisted boundary conditions, exists, remains an open question.

Despite the fact that an exact bosonization formula is not known for $\psi_L^{\dagger\alpha}\psi_{Rj\beta}$, such a formula *is* known¹² for the fifth interaction term in (6) since it is a chiral SU(2) singlet. It can be written as

$$[h^i_{\{i}h^j\}_{j}} \exp(i\sqrt{8\pi/n_c}\varphi) + \text{H.c.}] .$$

As expected, it only involves the charge and color bosons. We now expect that the three couplings involving φ and h : λ_1 , λ_3 , and λ_5 will produce a gap for these excitations. It is simplest to consider the case where λ_3 is initially larger than the other two couplings. It is marginally relevant (if it is negative as calculated above) and produces a gap $m \propto \exp(-\pi/n_c |\lambda|)$. We would then expect that the field h would obtain a vacuum expectation value $\langle h^i_j \rangle \propto m^x \delta^i_j$, where x is the scaling dimension¹⁰ of h [$=3/2(2+n_c)$]. If we simply replace h by its vacuum expectation value in the λ_5 term we obtain a $\cos[\sqrt{8\pi/n_c}\varphi]$ interaction for φ . This is relevant, having dimension $2/n_c$ and thus should produce a gap in the charge sector proportional to $\exp[-3\pi/4(2+n_c)(n_c-1)|\lambda|]$. We also expect that $\exp(i\sqrt{2\pi/n_c}\varphi)$ will get a vacuum expectation value set by this mass scale. Upon integrating out these massive fields, we are left with the $k=2s$ WZW model as the critical theory.

Since we do not have a bosonization formula for $\psi_L^{\dagger i\alpha}\sigma_{\alpha\beta}\psi_{Ri\beta}$ we cannot deduce the correct representation of the spin operators with the same degree of rigour as for $s = \frac{1}{2}$. However we would expect that the operator in the critical theory with the right quantum numbers of lowest scaling dimension should appear. This is $\text{trg}\sigma$, as for $s = \frac{1}{2}$.

We now turn to the behavior for arbitrary spin Hamiltonians and hence arbitrary values of the six Hubbard model coupling constants. Since the fourth and sixth interactions mix spin with color and charge, we do not expect the spin sector to be protected in general and all couplings should tend to flow toward large values. We are unable to bosonize the fourth and sixth interaction terms, in general. However in the special case $n_c=2$ we *can* bosonize the sixth term. This follows¹² because in this case this operator can be written as

$$(\lambda_5/2)\epsilon_{ij}\psi_L^{\dagger i\alpha}\psi_L^{\dagger j\beta}\psi_{Ri\alpha}\psi_{Rm\beta}\epsilon^{lm} .$$

It is invariant under the chiral SU(2) *color* symmetry in this special case of $n_c=2$. Thus it can be bosonized entirely in terms of the *spin* and charge bosons proportional to $[g^{\{\alpha}_{\alpha}g^{\beta\}_{\beta}} \exp(i\sqrt{4\pi}\varphi) + \text{H.c.}]$. If we assume that λ_5 is very small compared to the other couplings then we may integrate out the color and charge fields. Thus we replace the exponential above by its vacuum expectation value. This gives a relevant interaction in the $k=2$ WZW model. It has dimension, $x=1$. (This is, in fact,

the only relevant operator permitted by symmetry for $k=2$.)

In the general case of arbitrary s and arbitrary values of the six coupling constants, we would also expect to generate relevant operators in the WZW model. In fact, it was not really justified to keep only four fermion operators in the continuum limit. We should instead consider all allowed relevant operators at the WZW fixed point. Apart from the marginal current-current interaction, there are additional relevant operators^{10,11} that respect diagonal SU(2) and the $g \rightarrow -g$ inversion symmetry. These are the primary fields of the Kac-Moody and conformal algebra. They are classified by their spin quantum numbers under the left and right SU(2) symmetries. Primary fields exist with equal left and right spins j , equal to an arbitrary half-integer or integer such that $j \leq k/2$; their scaling dimension is $x = 2j(j+1)/(2+k)$. The restriction on the maximum value of j can be obtained from the free fermion theory. We can construct operators out of $2j \psi_L^\dagger$'s and $2j \psi_R$'s with left and right spin j . But these operators are zero due to Fermi statistics for $2j > n_c$. They correspond to $2j$ -fold products of the elementary field g (which has $j = \frac{1}{2}$). Thus only the integer j fields respect the inversion symmetry. Therefore there is a relevant operator respecting all symmetries of the generalized Hubbard model for each positive integer $j < k/2$ whose dimension $2j(j+1)/(2+k) < 2$. For large k the number of relevant operators, n_r , grows like \sqrt{k} .

Thus we should expect that if we adjust a number of parameters in the spin chain Hamiltonian equal to the number of relevant operators, then the critical theory will be the $k=2s$ WZW model. From this point of view, we see that the integrable Hamiltonians correspond to such special multicritical points. Why the integrable models should happen to be multicritical rather than generic remains an interesting and unanswered question. However since the number of possible nearest neighbor couplings is $2s = k$ we see that the integrable Hamiltonians are not the *only* such multicritical nearest-neighbor Hamiltonians but should lie in a space of dimension $2s - n_r$.

One might expect that the theories would develop a gap for generic Hamiltonians with $s > \frac{1}{2}$. After all, it was chiral symmetry which was protecting a massless sector for $s = \frac{1}{2}$ and at the multicritical points for general s . If this symmetry is broken by relevant operators why should there be *any* massless sector? The answer to this question is quite surprising. There appears to be a type of topological stability which protects a massless sector for odd n_c (half-odd-integer s) whereas for even n_c (integer s) there is in general a gap. To understand this, we consider the case of very large n_c . We will imagine that the relevant chiral symmetry breaking operators are small so that the system is flowing away from the $k = n_c$ fixed point. At large k , the WZW model becomes essentially a free theory, so a semiclassical analysis becomes justified. That is, writing $g = \exp(i\sigma \cdot \varphi/2)$, we may regard the triplet of bosons, φ , as being essentially free fields. Let us consider only the most relevant interaction, which can be written as

$$\mathcal{L}_{\text{int}} = -V = -\lambda(\text{tr}g)^2,$$

where V is the potential energy density. Let us analyze classically the effect of this operator. If $\lambda < 0$, then the minimum of V occurs at $g = \pm 1$ ($\varphi = 0$ or $|\varphi| = 2\pi$). Thus the discrete symmetry $g \rightarrow -g$ is spontaneously broken. Correspondingly, the spin chain is in a spontaneously dimerized phase with the symmetry of translation by one site spontaneously broken. Expanding V in powers of φ we obtain

$$V \approx \text{const} + |\lambda| \varphi^2 + \dots$$

Thus all three degrees of freedom obtain a mass proportional to $\sqrt{|\lambda|}$. The spontaneously dimerized phase has a mass gap.

On the other hand, if $\lambda > 0$, then the minimum of V occurs at $|\varphi| = \pi$, $g = i\sigma \cdot \hat{\varphi}$, where $\hat{\varphi} = \varphi/|\varphi|$. Note that diagonal SU(2) rotations

$$g_\alpha^\beta \rightarrow U_\alpha^\gamma g_\gamma^\delta U_\delta^\beta$$

transform φ by the corresponding SO(3) rotation

$$\varphi^i - R^i_j \varphi^j.$$

The minimum of V now occurs at an arbitrary point on the sphere and breaks the diagonal SU(2) symmetry. Correspondingly the rotational symmetry of the Hubbard model or spin chain is spontaneously broken, in this approximation. The longitudinal component of φ obtains a mass proportional to $\sqrt{\lambda}$ but the transverse components (the two angles parametrizing $\hat{\varphi}$) are massless Goldstone bosons in this semiclassical approximation. Let us go beyond the semiclassical approximation by considering the interactions between these would-be Goldstone bosons. Thus we integrate out the longitudinal part of φ . To lowest order we simply replace g by $i\sigma \cdot \hat{\varphi}$ in the WZW Lagrangian. The first term in S_{WZW} gives

$$\mathcal{L} = (k/4\pi) \partial_\mu \hat{\varphi} \cdot \partial^\mu \hat{\varphi}.$$

This is the Lagrangian of the O(3) σ model with coupling constant $2\pi/k \ll 1$. The interactions between these would-be Goldstone bosons as represented by the O(3) σ model, are expected to restore the symmetry and produce an exponentially small mass gap in (1+1) dimensions

$$m \propto \exp(-k).$$

Thus we expect that the transverse components will not be strictly massless for any finite k although they will be much lighter than the longitudinal component.

However this analysis is not yet complete, because we have neglected the effect of the Wess-Zumino term. It also makes a relevant contribution after integrating out the longitudinal fluctuations of φ . In fact freezing the magnitude of φ reduces the Π_3 topological term of the WZW model to the Π_2 topological term of the O(3) σ model. A simple way of seeing this is to write an extrapolation of the field g to the three-dimensional half-space as

$$g(x_\mu) = \exp[if(x_3)\sigma \cdot \hat{\varphi}(x_1, x_2)],$$

where f is any smooth function such that $f(-\infty)=0$ and $f(0)=\pi/2$. The Wess-Zumino term then becomes

$$\Gamma = 4iQ \int dx_3 (df/dx_3) \sin^2 f = i\pi Q,$$

where Q is the integer-valued Π_2 topological term,

$$Q \equiv (1/8\pi) \int d^2x \hat{\varphi} \cdot (\partial_\mu \hat{\varphi} \times \partial_\nu \hat{\varphi}) \epsilon^{\mu\nu}.$$

[The normalization can be checked by the following argument. A simple solitonlike configuration which has a Π_3 topological charge of one can be obtained by taking $\hat{\varphi}$ to be an instanton with $Q=1$, and $f(x_3)$, a smooth function that increases monotonically from 0 at $x_3=-\infty$ to $\pi/2$ at $x_3=0$ to π at $x_3=\infty$. Thus $g(x_3=-\infty)=1$, $g(x_3=0)=i\hat{\sigma}$, and $g(x_3=\infty)=-1$. The Wess-Zumino term is normalized to be $2\pi i$ times the half-space integral of the Π_3 topological charge density, in order that the ambiguity in Γ be $2\pi i$. But the half-space contains half the Π_3 topological charge in this particular case so $\Gamma=i\pi$ for an instanton with $Q=1$.]

Thus we see that the topological angle in the effective $O(3)$ σ model is $\theta=\pi k$. The physics is periodic in θ since the path integral contains the factor $\exp(i\theta Q)$ and Q is an integer. Thus θ is effectively zero for even k and π for odd k . The behavior of the $O(3)$ σ -model at $\theta=0$ is very well understood and one expects a gap as stated above.

Very little is known with certainty about the behavior at $\theta=\pi$ from standard field theory methods. It appears likely to be some sort of special singular point. In the large- n CP^n model¹³ [$O(3)$ corresponds to CP^1] there is a first-order phase transition at $\theta=\pi$. This corresponds to a spontaneous breaking of parity $x_1 \rightarrow -x_1$. (This symmetry is explicitly broken for all values of θ except 0 and π .) Instanton arguments⁶ suggest that in the case of the $O(3)$ model the mass gap may vanish at the point $\theta=\pi$.

The most insight into the behavior of this model comes from the study of quantum spin chains. It was argued⁶ that the $O(3)$ model is obtained as the low-energy theory of the Heisenberg spin Hamiltonian in the limit of large s , or of large ferromagnetic second nearest neighbor interactions. In fact one obtains this limit for a range of spin-chain Hamiltonians in which the spin-wave interactions are small. However this range does *not* include the large- s integrable models. In terms of the Hubbard model representation for $s=\frac{1}{2}$, a large ferromagnetic second nearest neighbor interaction corresponds to a large positive value of the marginally irrelevant coupling λ_2 ; one still expects the critical theory to be the $k=1$ WZW model. This suggests that the $O(3)$ model is indeed massless at $\theta=\pi$ and that the critical theory is the $k=1$ WZW model. Furthermore, generic half-odd-integer s spin chains should have this as the critical theory. A rigorous argument¹⁴ has been given that half-odd-integer s chains must have zero mass when they are in a phase with a unique ground state (no broken discrete symmetries). So we should expect that half-odd-integer s chains are generically either in the $k=1$ universality class or else in a dimerized phase (or possibly some other phase with degenerate ground-

states). On the other hand, for integer s we expect either a massive phase of unbroken symmetry [corresponding to the $O(3)$ σ model at $\theta=0$ for large s] or else a dimerized phase.

There is support for these arguments from numerical diagonalizations of finite chains. A gap has been seen¹⁵ for $s=1$ and critical exponents characteristic of the $k=1$ WZW model have been measured for generic $s=\frac{3}{2}$ Hamiltonians (whereas for the integrable Hamiltonian one sees $k=3$ exponents).⁷

Thus we conclude that the critical theory for a large odd- k WZW model with a negative $(\text{trg})^2$ interaction should be the $k=1$ WZW model. We should really not restrict ourselves to a single relevant interaction but include all relevant operators permitted by symmetry. The classical potential can in general be written as a periodic function of $|\varphi|$ only, due to the diagonal $SU(2)$ symmetry. It is also symmetric under $|\varphi| \rightarrow 2\pi - |\varphi|$ which corresponds to $g \rightarrow -g$. For some range of parameters we expect this discrete symmetry to be unbroken and the minimum to lie at $|\varphi|=\pi$. In this case the low-energy theory will be the $O(3)$ σ model as above. For odd k we then expect crossover to the $k=1$ fixed point. For another range of parameters, this discrete symmetry will be spontaneously broken and the system will generically develop a gap. This corresponds to a short-range dimerized phase of the quantum spin chain. It now seems very likely that crossover to the $k=1$ fixed point occurs for *any* odd k . The only role of large k in the above arguments was to make the transverse components of φ much lighter than the longitudinal component. The numerical simulations⁷ indicate that the above picture is correct for $k=3$.

We are thus led to the conclusion that in a large class of models there is a massless phase described by the $k=1$ WZW model. These models include half-odd-integer spin chains, generalized Hubbard (or, in the continuum limit) Thirring models with an odd number of colors, WZW models with odd k and the $O(3)$ σ model with $\theta=\pi$. It is not surprising that this should be the generic critical theory for $SU(2)$ invariant systems since it is the *only* WZW model in which there are no relevant operators.

We expect the phase diagram for a half-odd-integer s quantum spin chain to have a massless region in the $k=1$ universality class. Outside this region the system is presumably dimerized (or else goes into a ferromagnetic phase or possibly some more exotic phase). The multicritical points are likely to occur on the boundaries of the $k=1$ region. The simplest case is $s=\frac{3}{2}$. There is only one relevant operator $(\text{trg})^2$ and the marginal operator $\mathbf{J}_L \cdot \mathbf{J}_R$. Thus we can consider a two dimensional parameter space. The two parameters could be, for example, second-nearest-neighbor and biquadratic couplings. The anticipated phase diagram is shown in Fig. 1. One boundary of the massless phase is determined by the vanishing of the marginal coupling. Thus the mass should grow exponentially slowly upon crossing this boundary. It contains the flow line from the $k=3$ to the $k=1$ fixed points. The other boundary is determined by the relevant coupling vanishing. Thus the mass should

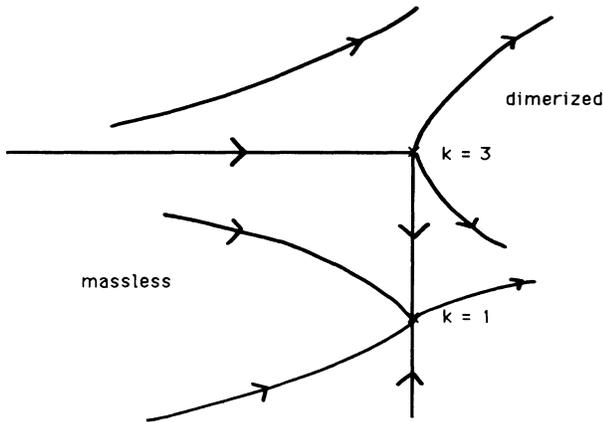


FIG. 1. Phase diagram for translation invariant $s = \frac{3}{2}$ chains or $k=3$ WZW models with $g \rightarrow -g$ symmetry.

have power-law growth upon crossing it. Points along this boundary are attracted to the $k=3$ fixed point. The integrable model presumably lies along such a boundary.

Integer- s chains should have a similar looking phase diagram except that the massless $K=1$ region is replaced by a massive region with unbroken symmetry. Outside this region exist dimerized phases (or ferromagnetic, etc.). The multicritical points presumably lie on the boundaries of the massive singlet phase. This seems to be consistent with numerical work on $s=1$ chains in the vicinity of the integrable point,¹⁶ and variational and large- N arguments.¹⁷

It seems likely that, for integer or half-odd-integer s , $k=2s$ is not the *only* multicritical point that can occur; other (lower?) values of $k > 1$ should also be possible.

Note that an *explicit* breaking of the discrete symmetry (staggered interactions in the spin chain) will shift the minimum of the potential away from $|\varphi| = \pi$ and thus shift the topological angle away from π (or zero). Repeating the above calculation, we find a topological angle $\theta = k(|\varphi| - \sin|\varphi|)$. Thus a symmetry-breaking operator like $\text{tr}(g)$ gains a topological significance in the low-energy theory. We expect shifting θ to produce a mass. It should lead to a $\text{tr}(g)$ term in the $k=1$ WZW model, of dimension $\frac{1}{2}$ and thus produce a gap $\propto |\theta - \pi|^{2/3}$ (up to logarithmic corrections). As we change the strength of the explicit symmetry breaking we should expect to pass through several phase transitions at point where $\theta = \pi \pmod{2\pi}$. For example, a semiclassical (mean-field) analysis of the potential

$$V = \lambda(\text{tr}g)^2 + \mu \text{tr}g \tag{9}$$

gives the phase diagram shown in Figs. 2 and 3. Figure 2 shows the regions where $|\varphi| = 0$ or 2π . In these regions the semiclassical spectrum is a massive triplet. Outside these regions it consists of one massive particle and two Goldstone bosons. Figure 3 shows the lines on which $\theta = \pi$ for $k=1,2,3$. As $|\varphi|$ varies between 0 and 2π , θ varies between 0 and $2\pi k$, passing through $\pi \pmod{2\pi}$ $2k-1$ times. It seems likely that this phase diagram is qualitatively correct even at the quantum lev-

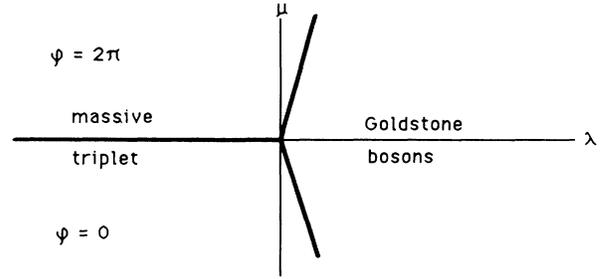


FIG. 2. Semiclassical phase diagram for the WZW model of (9) (ignoring topological and quantum effects).

el for finite k . There should be $2k-1$ second-order transition lines in the vicinity of which the $O(3)$ σ -model at $\theta = \pi$ is the correct critical theory. There is also one first-order line where the explicit symmetry breaking vanishes, separating equivalent phases (the negative λ axis). Altogether there are $2k$ phases. These can be

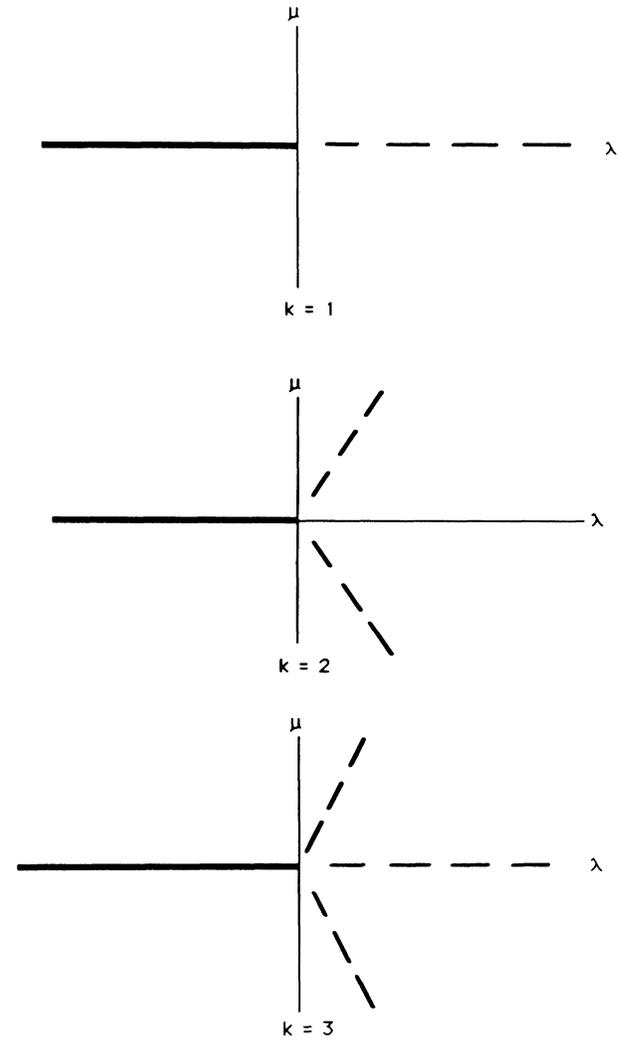


FIG. 3. Transition lines where $\theta = \pi$ (in the semiclassical approximation) for the WZW model of (9) for $k=1,2,3$.

thought of as having different degrees of dimerization. Pairs of phases are mapped into each other by the discrete symmetry with only the totally undimerized phase (which exists only for even k or integer s) being unique. [The semiclassical phase boundaries separating the "massive triplet" regions from the "Goldstone bosons" region in Fig. 2 are presumably not true phase boundaries in the quantum theory. However, at large k , the mass of the transverse modes of φ changes from $O(1)$ to $O(\exp(-k))$ close to these lines.] Precisely such a phase diagram was found in the large- n limit of quantum spin chains.¹⁷

The present analysis complements several other approaches to quantum spin chains. The argument⁶ that at large- s , the low-energy spectrum of a quantum spin chain is described by the $O(3)$ σ model with $\theta=2\pi s$ is now seen to be true in a finite region in the space of spin Hamiltonians. It fails at the multicritical points and in the dimerized regions. Moving even infinitesimally away from one of the multicritical points into the undimerized region, it is again true. The, in many ways unfortunate, fact that the integrable models are examples of such multicritical points no longer appears to be a counter example to the field-theory arguments. Likewise, the Abelian bosonization approach to higher- s chains¹⁸ which predicts generic $k=1$ critical behavior for half-odd-integer s is also substantiated by this analysis of the vicinity of the multicritical points.

Furthermore, the conclusion that the critical theory for the $O(3)$ σ model at $\theta=\pi$ is the $k=1$ WZW model is consistent with a recent theorem of Zamolodchikov.¹⁹ This theorem states that if a field theory flows between two conformally invariant fixed points then the value of the conformal anomaly parameter c must be smaller at the infrared stable fixed point. In this case the flow is from the unstable zero-coupling fixed point of the σ model to the $k=1$ fixed point. The unstable fixed point is a theory of two free (Goldstone) bosons with $c=2$; the stable fixed point has $c=1$.

Standard field-theory methods: Monte Carlo²⁰ and the large- n limit,¹³ have apparently not been very successful in studying the $O(3)$ σ model near $\theta=\pi$. Obtaining it

from the odd $k \rightarrow \infty$ limit of the WZW model provides a useful field-theory definition of the model. A lattice regularization of the WZW models is then provided by spin chains in the vicinity of the integrable points. Such models can be studied very successfully by numerical methods of a different character than those normally used in field theory. Namely, since the Hilbert space is finite dimensional for a finite chain, exact diagonalization can be used. The work on $s=\frac{3}{2}$ provides rather compelling evidence⁷ that the $O(3)$ σ model is indeed massless at $\theta=\pi$. Of course, the limit of large k (i.e., large s) presents difficulties. An alternative approach is to study the $s=\frac{1}{2}$ chain with a large ferromagnetic second-nearest-neighbor interaction.

There are not many known mechanisms in field theory (or in condensed matter physics) that will guarantee the stability of massless excitations in the presence of interactions. In four dimensions these include gauge invariance (which leads to a massless photon), spontaneous symmetry breaking (which leads to massless Goldstone bosons) and chiral symmetry (which if unbroken can, in some cases lead to massless fermions by the 'tHooft anomaly conditions). In two dimensions a massless phase can arise as a result of Abelian or non-Abelian chiral symmetry. In some field theories this symmetry is exact. In other cases (including all the condensed matter systems) it is not an exact symmetry of the microscopic model but is an effective symmetry of the critical theory, being broken only by irrelevant operators. The above arguments suggest that a topological mechanism plays a role in determining which Hamiltonians are attracted to the chirally invariant fixed point.

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