Spin-*s* wave functions with algebraic order

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We generalize the Gutzwiller wave function for $s=\frac{1}{2}$ spin chains to construct a family of wave functions for all $s>\frac{1}{2}$. Through numerical simulations, we demonstrate that the spin spin correlation functions for *all s* decay as a power law with logarithmic corrections. This is done by mapping the model to a classical statistical mechanical model, which has coupled Ising spin chains with long range interactions. The power law exponents are those of the Wess Zumino Witten models with $k=2s$. Thus these simple wave functions reproduce the spin correlations of the family of Hamiltonians obtained by the Algebraic Bethe Ansatz.

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I. INTRODUCTION

Quantum spin chains with power law correlations are of great current interest. Starting with the Bethe chain,[1] it has been known for a long time that half integer spin systems generically have spin correlation functions that decay as the inverse of the distance between the spins. For integer spin chains, the correlation functions are generically expected to decay exponentially, due to the Haldane conjecture.[2] However, it is also known that special models can be constructed for which the spin correlation functions decay as a power law for all (including integer) spin *s*, with an exponent that depends on *s*. These models are realized from the Bethe Ansatz in its algebraic form. The work of the Leningrad school has provided concrete realizations, e.g., the model of Takhtajan and Babudjan[3] for spin 1. It has also provided a general technique for obtaining the Hamiltonian for all values of spin, starting from the Algebraic Bethe Ansatz.[4]

The coefficients of the biquadratic and other terms need to be specially chosen to obtain these models. Alternatively, the Algebraic Bethe Ansatz method automatically generates these Hamiltonians. The general construction of a field theory for these models was undertaken by Affleck,[5] who showed that these models belong to the Wess Zumino Witten (WZW) class. These models are characterized by a single parameter *k*, which determines the exponents. In this case, *k* turns out to be 2*s* for spin *s*. From the known behavior of the WZW theories, Affleck showed that the spin spin correlations are asymptotically of the form

$$|\langle \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j \rangle| \sim |i-j|^{-3/(2s+2)}. \tag{1}$$

For any *s*, the field theory has a marginal operator in the renormalization group sense. This gives rise to a multiplicative factor[6] of $[A+B\ \ln|i-j|]^{1/2}$ in the correlation function of Eq. (1), unless the bare value of the marginal operator is fortuitously equal to its fixed point value.[7,8]

An alternative recent line of thought has been to study explicit wave functions. In particular, the Gutzwiller wave function in one dimension has been very successful. The Gutzwiller wave function takes the free fermion determinantal wave function and retains all configurations with single occupancy of electrons. Thus at half filling, i.e., one electron per site, it yields a wave function that has only spin degrees of freedom. This insulating spin wave function inherits the power law correlations of the parent free Fermi wave function, albeit with some renormalization of the values of the exponents. The work of Haldane,[7] Shastry,[8] and others[9] showed that the wave function is the exact ground state of a long ranged $s=1/2$ Heisenberg model that is in the same universality class as the Bethe chain, i.e., has the same correlation exponents.

In this paper, we propose a natural extension of the Gutzwiller wave function to obtain wave functions for *all s*, which (based on our numerical results) seem to have power law correlations of the form in Eq. (1). Thus we have constructed for wave functions the analog of the Algebraic Bethe Ansatz method for Hamiltonians: a prescription that yields the nongeneric correlations of Eq. (1) automatically, i.e., without any fine tuning of parameters. This paper builds on ideas presented earlier in Ref. 10.

We start with 2*s* copies of the Gutzwiller wave function, and use the principle of symmetrization to produce an angular momentum $J=s$ wave function, i.e., one where each lattice site has a spin *s* degree of freedom. Symmetrization is a well known procedure in angular momentum theory, where one generates the states of a spin *J* system by taking 2*J* copies of spin half states and projecting out all states that are not fully symmetric in the 2*J* spin constituents. This procedure clearly generates wave functions for particles of angular momentum *s*. Based on the experience with $s=1/2$, one would hope that these wave functions might also inherit the power law correlations of the parent free Fermi gas, again with some as yet undetermined renormalization of values of exponents.

We are able to perform the symmetrization of this wave function explicitly, using the elegant formalism of spin coherent states. We further study the properties of this wave function using numerical techniques. When the wave function is squared, it can be conveniently interpreted as a statistical mechanical model of 4*s* parallel chains of logarithmically interacting particles with certain couplings, i.e., a generalization of the Wigner Dyson Coulomb problem. Our numerical results for $s=1,3/2,2$ are presented here. Together with the analytically known results for $s=1/2$, they support the remarkable conclusion that these wave functions provide a *lattice realization* of the WZW models with $k=2s$.

We are unable to address the issue of finding a Hamiltonian for which the states here are exact ground states, but

have wave functions that are explicit and rather beautiful. This seems to be just the opposite situation of the Algebraic Bethe Ansatz models[4] for higher spin, where the Hamiltonians are relatively straightforward, but the wave functions are highly complicated.

Earlier numerical work by Shastry[10] on the same wave function for $s=1$, with relatively shorter spin chains, gave results that were consistent with the same exponents as found here, but lacked the resolution to determine the logarithmic corrections to the leading behavior. We note that spin coherent states were used for a similar mapping of spin wave functions to statistical mechanical problems in the work of Arovas, Auerbach, and Haldane[11] as well as Affleck, Kennedy, Lieb, and Tasaki (AKLT), who studied the $s=1$ model of AKLT,[12] for which correlations are exponential. The calculation of the correlations is considerably easier than in the cases studied here. AKLTs method of solution is also a very nice application of the idea of symmetrization that we use in the present paper. Analytical and numerical results for the spin-half chain, with the corresponding statistical mechanical model studied as a function of temperature, have been presented earlier.[13]

II. SPIN COHERENT STATES, SYMMETRIZATION, AND THE GUTZWILLER WAVE FUNCTION

A. Spin coherent states

We begin by recapitulating the salient definitions of spin coherent states. There are several related variants of these, and each has slightly different advantages. Let us consider a single site. The functions introduced by Radcliffe[14] are defined for angular momentum J as

$$|\Omega\rangle = e^{[S^- \exp(i\phi) - S^+ \exp(-i\phi)]\theta/2}|J\rangle = \cos^{2J}(\theta/2) e^{\tan(\theta/2)\exp(i\phi)S^-}|J\rangle$$
$$= \sum_{n=0}^{2J} \{{}^{2J}C_n\}^{1/2} \cos^{2J-n}(\theta/2)\sin^n(\theta/2)e^{in\phi}|J-n\rangle. \quad (2)$$

Radcliffe also introduced a related set of states,

$$|z\rangle_R = e^{zS^- - z^*S^+}|J\rangle. \quad (3)$$

These are normalized and related to the first set by setting $z \to \tan(\theta/2)e^{i\phi}$. Another set of coherent states were found to be very convenient[15] for the purpose of obtaining differential operator representations of spin operators, e.g., $S^z \to (s - z^* \partial/\partial z^*)$ in the space of "wave functions" $\langle z|\psi\rangle$. These coherent states were the unnormalized states

$$|z\rangle = e^{zS^-}|J\rangle = \sum_{n=0}^{2J} \{{}^{2J}C_n\}^{1/2}(z)^n|J-n\rangle, \quad (4)$$

with $|z\rangle_R = (1+|z|^2)^{-J}|z\rangle$. The relationship between the wave functions $\psi(z^*) \equiv \langle z|\psi\rangle$, $\psi_R(z^*) \equiv {}_R\langle z|\psi\rangle$ and $\psi(\Omega^*)$ follows from the relationship between the basis functions, we note the relation needed later:

$$\psi(\Omega^*) = \cos^{2J}(\theta/2)\psi(z^*) \quad \text{with } z^* \to \tan(\theta/2)e^{-i\phi}. \quad (5)$$

The functions $\psi(z^*)$ are polynomials in z^* of maximal degree $2J$, and lend themselves to very simple "symmetrization" rules that we discuss in the next subsection of this paper.

Next, we need to construct the rules for obtaining averages of variables in states. We begin by noting the diagonal representation of an arbitrary operator A[16] followed by its average as:

$$A = \frac{(2J+1)}{4\pi}\int d\Omega\ a(\Omega)|\Omega\rangle\langle\Omega|, \quad (6)$$

where the prefactor has been chosen so that $a(\Omega)=1$ for the identity operator. To compute averages, we write

$$\langle\psi|A|\psi\rangle = \frac{(2J+1)}{4\pi}\int d\Omega\ a(\Omega)\langle\Omega|\psi\rangle\langle\psi|\Omega\rangle$$
$$= \frac{(2J+1)}{4\pi}\int d\Omega\ a(\Omega)|\psi(\Omega)|^2. \quad (7)$$

Thus, given a wave function $\psi(\Omega^*) \equiv \langle\Omega|\psi\rangle$, we can find the expectation value of any operator if its $a(\Omega)$ is known. For future reference, we note that $a(\Omega)$ for the operator S_z is $(J+1)\cos\theta$. An important corollary that we will use is that if spin coherent states are constructed for every site in a lattice, the expectation value of an operator $\langle A_i B_j\rangle$ can be found by using the corresponding weight function $a(\Omega_i)b(\Omega_j)$ in the integrals, where $a(\Omega)$ and $b(\Omega)$ are the functions for isolated sites. This will be used for the spin correlation function.

B. Symmetrization

Let us consider a simple case of two spin $\frac{1}{2}$ particles with

$$|\phi\rangle = \alpha_1\beta_2. \quad (8)$$

Symmetrization is best understood from its action on states, so in the present case

$$S|\phi\rangle = \tfrac{1}{2}(\alpha_1\beta_2 + \alpha_2\beta_1). \quad (9)$$

On more general functions of many copies of spin half, its action is similarly defined, namely find the fully symmetric combination generated from a seed state and divide by the total number of generated states. We next deduce the rule for symmetrizing $2s$ copies of spin $1/2$ in the space of coherent state wave functions. It turns out that the most efficient way is to work with the unnormalized coherent states Eq. (4) where the wave functions are just polynomials in z^*. Let us label the $2s$ copies of spin $1/2$ by $z^*(\alpha)$ and the resulting spin s variables by Z, so that a coherent states of the direct product states and the final spin s state are

$$|\{z(1),z(2)\ldots z(2s)\}\rangle = \prod_{\alpha=1}^{2s}(|1/2\rangle_\alpha + z(\alpha)|-1/2\rangle_\alpha), \quad (10)$$

$$|Z\rangle = \sum_{m=0}^{2s}\{{}^{2s}C_m\}^{1/2}(Z)^m|2s-m\rangle. \quad (11)$$

Generic states in the direct product space and the final spin s space are represented by $|\phi\rangle$ and $|\Phi\rangle$, respectively, and the role of symmetrization is to map the former into the latter as

$$\mathcal{S}|\phi\rangle = |\hat{\phi}\rangle,$$

$$|\hat{\phi}\rangle \leftrightarrow |\Phi\rangle. \tag{12}$$

The question we address is: given a state $|\phi\rangle$, what is the resulting state $|\Phi\rangle$ for the spin $2s$ particle. The answer turns out to be remarkably simple in the unnormalized coherent state basis. If we denote

$$f\big[\{z^*(1), z^*(2)\ldots z^*(2s)\}\big] = \langle\{z^*(1), z^*(2)\ldots z^*(2s)\}|\phi\rangle,$$

$$\hat{f}\big[\{z^*(1), z^*(2)\ldots z^*(2s)\}\big] = \langle\{z^*(1), z^*(2)\ldots z^*(2s)\}\mathcal{S}|\phi\rangle,$$

$$F(Z^*) = \langle Z^*|\Phi\rangle, \tag{13}$$

we find (and demonstrate later) that

$$F(Z^*) = f(Z^*, Z^*\ldots Z^*). \tag{14}$$

This implies that by ignoring the distinction between the different copies of the spin $1/2$ and replacing every occurrence of $z^*(\alpha)$ by Z^* gives us a coherent state representative of the spin s particle. This result is obvious for the special (symmetric) cases of $f=1$ and$f=\Pi z^*(\alpha)$, but not so obvious for other cases, since one has to rule out possible nontrivial dependence on the degree of the polynomial.

We now give a brief proof of this assertion. It suffices to consider the general case of a polynomial of degree r, thus

$$f = z^*(1)z^*(2)\ldots z^*(r),$$

$$\hat{f} = \frac{r!\,(2s-r)!}{2s!} \sum_{1\leqslant i_1\langle i_2\ldots\langle i_r\leqslant(2s)} z^*(i_1)z^*(i_2)\ldots z^*(i_r). \tag{15}$$

The state $\hat{f}$ clearly is proportional to the state deriving from $(S^-)^r|J_z=2s\rangle$, the proportionality constant is readily worked out so

$$|\Phi\rangle = \frac{(2s-r)!}{(2s)!}(S^-)^r|2s\rangle, \tag{16}$$

hence,

$$F(Z^*) = (Z^*)^r\left\{\frac{(2s-r)!}{(2s)\ !\,r!}\langle 2s|(S^+)^r(S^-)^r|2s\rangle\right\} = (Z^*)^r. \tag{17}$$

The last line follows on using the commutation relations of angular momentum.

C. Gutzwiller type wave functions

The Gutzwiller wave function for a one dimensional Fermi gas at half filling is expressible in the form[8]

$$\begin{aligned}|\psi_G\rangle &= \mathcal{N}\prod_{j=1}^{L}[1-n_{j,\uparrow}n_{j,\downarrow}]\prod_{|k|\leqslant k_F} c^\dagger_{k,\uparrow}c^\dagger_{k,\downarrow}|0\rangle \\ &= \mathcal{N}\sum_{1\leqslant r_1\langle\ldots\langle r_n\leqslant L} e^{\{i\pi\Sigma_j r_j\}}\left\{\prod_{k\langle j}\sin^2\big[\pi(r_j-r_k)/L\big]\right\} \\ &\quad\times S^-_{r_1}S^-_{r_2}\ldots S^-_{r_n}|L/2\rangle\end{aligned} \tag{18}$$

with $n=L/2$. Here $c^\dagger_k$ is a creation operator with wave vector k in the original Fermionic representation, and the $[1-n_{j,\uparrow}n_{j,\downarrow}]$ factors ensure no double occupancy for any site j. S^- are the spin lowering operators in the spin representation that is equivalent at half filling. $\mathcal{N}$ is the normalization that we will not specify till the end, since it cancels out in the evaluation of the correlations. For simplicity we have confined our considerations to the case of $L/2$ overturned spins, so we are dealing with a global singlet wave function, made up of L spin $1/2$ particles.

We next consider $2s$ copies of this wave function, and project into the spin s sector at each site. In view of the discussion in the last section, this is most easily done with the coherent state notation, so the product wave function is written down directly as

$$\begin{aligned}&\Psi(Z^*_1, Z^*_2, \ldots Z^*_L) \\ &\quad= \mathcal{N}\Big[\sum_{1\leqslant r_1\langle\ldots\langle r_{L/2}\leqslant L} e^{\{i\pi\Sigma_j r j\}}\left\{\prod_{k<j}\sin^2\big[\pi(r_j-r_k)/L\big]\right\} \\ &\qquad\times Z^*_{r_1}Z^*_{r_2}\ldots Z^*_{r_{L/2}}\Big]^{2s}.\end{aligned} \tag{19}$$

To obtain this result, we wrote $|\psi_G\rangle$ in terms of $z^*(\alpha)$, multiplied $2s$ copies of this, and then symmetrized the wave function by dropping the distinction between the different copies or replicas. To reconstruct the wave function in the angular basis we use Eq. (5) and write

$$\Psi(\Omega^*_1, \Omega^*_2\ldots\Omega^*_L) = \prod_{j=1}^{L}\cos^{2s}(\theta_j/2)\Psi(Z^*_{r_1}, Z^*_{r_2}\ldots Z^*_{r_{L/2}}). \tag{20}$$

In order to make this more tractable, we introduce "occupation numbers" ρ^α_j which determine whether we get a $\cos(\theta_j/2)$ or $\sin(\theta_j/2)$ factor at a given site j in a particular "replica" α. Thus at each site we get a factor of

$$\begin{aligned}\text{factor} &= \prod_{\alpha=1}^{2s}[\cos(\theta_j/2)(1-\rho^\alpha_j) + \sin(\theta_j/2)e^{-i\phi_j+i\pi j}\rho^\alpha_j] \\ &= \cos^{2s}(\theta_j/2)\exp\left[\sum_{\alpha=1}^{2s}\rho^\alpha_j\ln\{\tan(\theta_j/2) + i\pi j - i\phi_j\}\right].\end{aligned} \tag{21}$$

We thus write the wave function as

$$\begin{aligned}&\Psi(\Omega^*_1, \Omega^*_2\ldots\Omega^*_L) \\ &\quad= \mathcal{N}\prod_{j=1}^{L}\cos^{2s}(\theta_j/2)\sum_{\{\rho^\alpha_j=0,1\}}{}' \\ &\quad\times\exp\left\{\sum_{\alpha=1}^{2s}\left[\sum_{j<k}\rho^\alpha_j\rho^\alpha_k\ln\sin^2\frac{\pi(k-j)}{L}\right.\right. \\ &\qquad\left.\left.+\sum_j\rho^\alpha_j\ln\tan\frac{\theta_j}{2} + i\pi j - i\phi_j\right]\right\}.\end{aligned} \tag{22}$$

The sum over the occupancy integers ρ^α is constrained to obey $\Sigma_n\rho^\alpha_n = L/2$ for each replica α. In the next section we

continue the discussion of expectation values and correlation functions, which require taking the modulus square of this wave function.

III. COUPLED ISING REPRESENTATION

The probability density is $|\Psi(\{\Omega_1^*\ldots\Omega_L^*\})|^2$, so we need to multiply Ψ in Eq. (23) with its complex conjugate, leading to $4s$ replicas in all. The correlation function $\langle s_j^z s_k^z\rangle$ can be found by calculating $(s+1)^2\langle\cos\theta_j\cos\theta_k\rangle$ with this probability density, as noted after Eq. (7). From the fact that $|\Psi\rangle$ is a singlet state, this correlation function suffices to determine all components $\langle s^\alpha s^\beta\rangle$. The angular variables θ and ϕ can be integrated over, leaving only the ρ_j's. The problem reduces to one of interacting lattice gas particles.

Integration over the azimuthal angle ϕ_j can be done at each site j, and gives a constraint that $\Sigma_\alpha\rho_j^\alpha=\Sigma_{\alpha'}\rho_j^{\alpha'}\equiv s-m_j$, where α and α' refer to replicas in Ψ and Ψ^*, respectively. Note that the oscillating phase factor can be dropped in view of the constraint from the azimuthal integration.

The integral over θ_j is next performed

$$\int_0^\pi\left(\sin\frac{\theta_j}{2}\right)^{2s-2m}\left(\cos\frac{\theta_j}{2}\right)^{2s+2m}\sin\theta_j d\theta_j=2\frac{(s+m)!\,(s-m)!}{(2s+1)!}$$
$$=2W_s(m), \tag{23}$$

with the function $W_s(m)$ defined by this equation. For the spin autocorrelation function $\langle s_j^z s_k^z\rangle$, we have to insert an extra factor of $(s+1)\cos\theta$ in the θ integrals at j and k. It is easy to verify that

$$(s+1)\int_0^\pi\left(\sin\frac{\theta_j}{2}\right)^{2s-2m}\left(\cos\frac{\theta_j}{2}\right)^{2s+2m}\cos\theta_j\sin\theta_j d\theta_j$$
$$=2mW_s(m). \tag{24}$$

The final result is like a classical partition function

$$Z=|\Psi(\{\Omega_1^*\ldots\Omega_L^*\})|^2$$
$$=\mathcal{N}\sum_{\rho_j^\alpha,\rho_k^{\alpha'}}\exp\left\{\sum_{j<k}\rho_j^\alpha\rho_k^\alpha\ln\sin^2[\pi(j-k)/L)]\right.$$
$$\left.+\sum_{j<k}\rho_j^{\alpha'}\rho_k^{\alpha'}\ln\sin^2[\pi(j-k)/L]\right\}\prod_j W_s(m_j), \tag{25}$$

where α and α' refer to replicas in Ψ and Ψ^*, respectively, $m_j=s-\Sigma_\alpha\rho_j^\alpha$ and the sum in the partition function Z is subject to the constraints

$$\sum_j\rho_j^\alpha=\sum_j\rho_j^{\alpha'}=L/2,$$
$$\sum_\alpha\rho_j^\alpha=\sum_{\alpha'}\rho_j^{\alpha'}. \tag{26}$$

When calculating the spin autocorrelation function $\langle s_j^z s_k^z\rangle$, the summation in Eq. (26) for Z is evaluated with an extra factor of $m_j m_k$.

It is convenient to change variables to $\sigma_j^\alpha=2\rho_j^\alpha-1$ and $\sigma_j^{\alpha'}=1-2\rho_j^{\alpha'}$. We then have $4s$ coupled Ising chains ($2s$ from Ψ and $2s$ from Ψ^*). The constraint Eq. (27) is equivalent to the condition that the sum of the Ising spins (not to be confused with the original quantum spins) across the different chains at any site must be zero. In addition, we impose the condition that the sum of the spins along any chain must be zero. With this condition, the interactions along any chain are

$$\sum_{j<k}\frac{1+\sigma_j^\alpha}{2}\frac{1+\sigma_k^\alpha}{2}\ln\sin^2\left[\pi(j-k)/L\right]$$
$$=\text{const}+\sum_{j<k}\frac{1}{4}\sigma_j^\alpha\sigma_k^\alpha\ln\sin^2\left[\pi(j-k)/L\right]. \tag{27}$$

The interactions along any chain are antiferromagnetic and logarithmic. The interaction across the different chains at any site occurs, apart from the constraint, through the $W_s(m)$ factor.

For the case of $s=1$, there is an alternative form of the partition function that is more convenient. With the constraint that the spins on the four chains at any site must add up to zero, there are six possible configurations at any site: (1,1,−1,−1), (1,−1,1,−1), (1,−1,−1,1), and the mirror images of these three. The magnetization m is 1 for the first and zero for the next two configurations. A remarkable simplification occurs once we note that $\Sigma_\alpha\sigma_j^\alpha\sigma_k^\alpha F(j-k)$ is equal to zero for any function F unless the configurations at the sites j and k are either identical or mirror images. (In the sum over α, the two replicas from ψ_s and the two from ψ_s^* are included.) Thus instead of four coupled Ising chains, the problem reduces to a six state Potts model on one chain. The states are labeled by $q=\pm1,2,3$. The configuration (1,1,1,1) is labeled with $q=1$, so that $m_j=\pm1$ when $q_j=\pm1$, and $m_j=0$ when $q_j=\pm2,\pm3$.The partition function is

$$Z\propto\sum_{q_1\ldots q_L}\exp\left\{\sum_{j<k}(\delta_{q_j,q_k}-\delta_{q_j,-q_k})\ln\sin^2[\pi(j-k)/L]\right\}$$
$$\times\prod_j(1+\delta_{q_j^2,1}). \tag{28}$$

The last factor comes from the fact that $W_s(\pm1)=2W_s(0)$. Two sites only interact with each other if their q's are identical or opposite. The condition that the total magnetization for each of the four original chains must be zero reduces to the statement that

$$\sum_j\delta_{q_j,n}=\sum_j\delta_{q_j,-n} \tag{29}$$

for any n.

Potts models can similarly be constructed for $s>1$, although they are more complicated: two sites j and k interact even when $q_j\neq\pm q_k$, and the condition from the total magnetization is weaker than Eq. (30). The numerical simulations reported in the next section were conducted with both the coupled Ising and the Potts representations.

IV. NUMERICAL RESULTS

Monte Carlo simulations were performed on the Ising and Potts representations given by Eqs. (26) and (29). For the

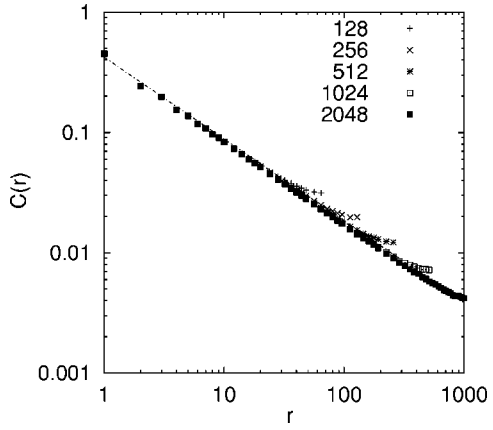

FIG. 1. Log-log plot of $C(r)$, the magnitude of the spin autocorrelation function, as a function of r for $s=1$. System sizes ranging from $L=128$ to $L=2048$ are plotted. The error bars are comparable to the point size. The data are consistent with a power law form, with exponent -0.68. Since logarithmic corrections are expected, a scaling collapse is not shown.

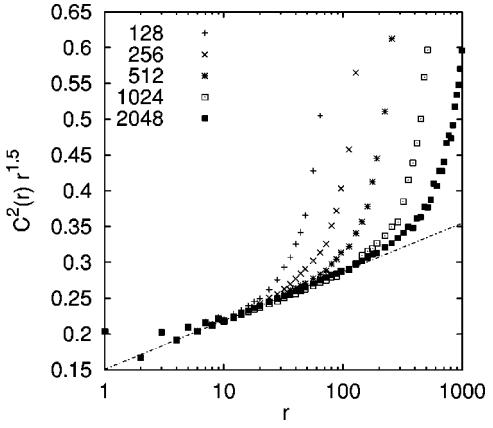

FIG. 2. Plot of $C^2(r)r^{1.5}$ as a function of $\ln r$ for $s=1$. This is predicted to be a straight line, with finite size corrections. System sizes from $L=128$ to $L=2048$ are plotted. The error bars are comparable to the point size.

Ising case, the constraint that the total spin along any chain and for all replicas at a site must be zero prevents using single spin flip dynamics. In a Monte Carlo move, two replicas (α,β) on two adjacent sites (j,k) were chosen at random. If the Ising spins at these four locations satisfy $\sigma_j^\alpha = \sigma_k^\beta$, $\sigma_j^\beta = \sigma_k^\alpha$, and $\sigma_j^\alpha \neq \sigma_j^\beta$, it is possible to flip all the four spins simultaneously without violating the constraint. The ratio of the probability of the flipped configuration to the probability of the unflipped configuration is calculated, with appropriate factors of $W_s(m)$ included if the move would change the magnetization at the sites, i.e., if $\alpha \leqslant 2s < \beta$ or $\beta \leqslant 2s < \alpha$. The move is accepted or rejected using the standard Metropolis criterion.

For the Potts representation, two adjacent sites (j,k) were chosen at random, and (q_j,q_k) were attempted to be changed. For the case of $s=1$, Eq. (30) required that if $q_j+q_k \neq 0$, the only possible move was to exchange them, while if $q_j+q_k=0$, one could attempt to replace them with either of the other two pairs of q values. For $s>1$, a table was constructed at the beginning of the numerical simulation. For any pair of q values (q_1,q_2), the table listed all pairs (q_1',q_2') that (q_1,q_2) could change to, while respecting the magnetization constraints on the underlying Ising spins. In any Monte Carlo step, this table was used to randomly select an allowable move to attempt. For both the Ising and the Potts representations, the long range logarithmic interaction down the chains made calculating the probability of an attempted move an $O(L)$ long calculation for a chain of length L. As a result, very large values of L could not be simulated.

In both cases, error bars on the measured correlation function were estimated by taking blocks of 30 000 readings, calculating the average correlation function within each block and then the interblock variance. Even if the individual readings are taken too frequently and are therefore correlated, this procedure should be reliable so long as the blocks are sufficiently large to be uncorrelated. It is also useful to compare the variance of the block averages to the variance of the individual readings within a block. The latter would be 30 000 times the former if the readings were uncorrelated. For our simulations, the actual ratio ranged from about 30 000 to 300, confirming that in all cases the blocks are uncorrelated even when the individual readings are not.

Figure 1 shows the spin autocorrelation function $C(r) = (-1)^r \langle s_j s_{j+r} \rangle$ as a function of r for different L, for $s=1$. The antiferromagnetic interaction down the chains causes the oscillatory $(-1)^r$ factor. It is clear from the figure that the correlation function does not decay exponentially. As seen in the figure, the autocorrelation function seems to decay as $1/r^\mu$ with $\mu \approx 0.68$. However, motivated by the analytical considerations discussed in Sec. I, we try the functional form

$$C(r) = [A + B \ln r]^{1/2} \frac{1}{r^\mu} \tag{30}$$

with $\mu=0.75$. This is because the power-law part of $C(r)$ should scale as $\sim 1/r^\mu$ with $\mu = 3/(2s+2) = 0.75$ for $s=1$, with possible logarithmic corrections from the marginally ir-

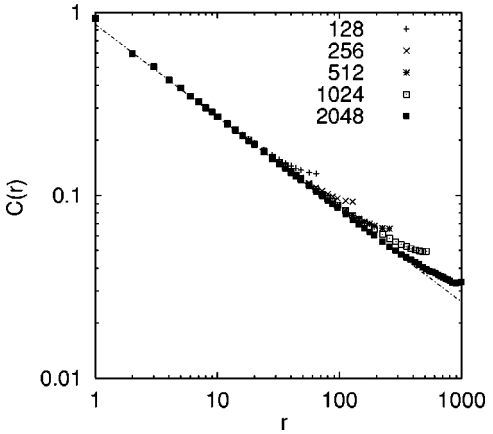

FIG. 3. Log-log plot of $C(r)$, the magnitude of the spin autocorrelation function, as a function of r for $s=3/2$. System sizes ranging from $L=128$ to $L=2048$ are plotted. The error bars are comparable to the point size. The data are consistent with a power law form, with exponent -0.51.

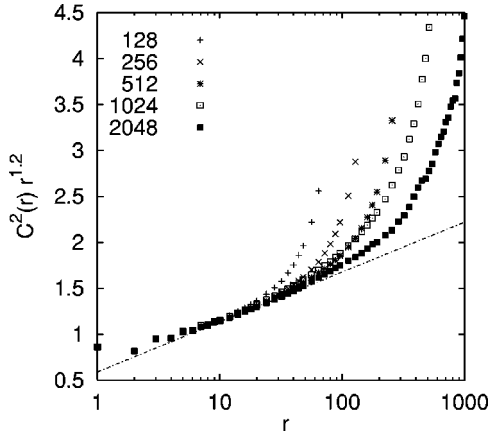

FIG. 4. Plot of $C^2(r)r^{1.2}$ as a function of $\ln r$ for $s=3/2$. System sizes from $L=128$ to $L=2048$ are plotted. The error bars are comparable to the point size.

relevant operator. Accordingly, Fig. 2 plots $C^2(r)r^{1.5}$, which should be a linear function of $\ln r$. This expectation is borne out by the plot. Logarithmic dependences are known to be hard to distinguish from weak power laws, and the plots cannot be used to choose between Eq. (31) and the pure power law decay of Fig. 1. [It would be even harder for the data to discriminate between more subtle differences, e.g., Eq. (31) with different exponents to the logarithmic term in the numerator.] However, from Fig. 2, the data are certainly in agreement with the analytical expectation.

Figures 3 and 4 are the counterparts of Figs. 1 and 2, respectively, for $s=3/2$. Based on the analytical prediction, Fig. 4 plots $C^2(r)r^{1.2}$ as a function of $\ln r$, since the power law decay part of $C(r)$ should have an exponent of $\mu=3/(2s+2)=0.6$. Likewise, Figs. 5 and 6 are for $s=2$, with $C^2(r)r^{1.0}$ plotted in Fig. 6. Although the results for $s=3/2$ and $s=2$ are not as clear as those for $s=1$, we see that $C(r)$ definitely does not decay exponentially for $s=2$, or as $\sim 1/r$ for $s=3/2$, the generic behavior expected for integer and

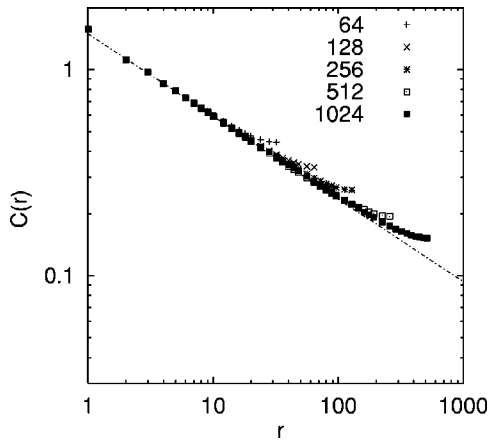

FIG. 5. Log-log plot of $C(r)$, the magnitude of the spin autocorrelation function, as a function of r for $s=2$. System sizes ranging from $L=64$ to $L=1024$ are plotted. The error bars are comparable to the point size. The data are consistent with a power law form, with exponent -0.40.

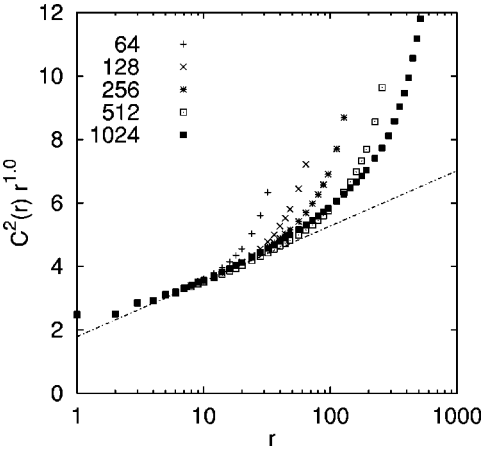

FIG. 6. Plot of $C^2(r)r^{1.0}$ as a function of $\ln r$ for $s=2$. System sizes from $L=64$ to $L=1024$ are plotted. The error bars are comparable to the point size.

half-integer spin chains, respectively. The decay of $C(r)$ is consistent with the expectation that each s corresponds to a WZW model of order $k=2s$. The effective μ's from Figs. 3 and 5 are 0.51 and 0.40, respectively.

Since there is no clear linear region in Fig. 6, we also plot the data in a manner that eliminates finite size effects. For finite system size L, the leading effect on $C(r)$ is to change its form from Eq. (31) to

$$C(r) = [A + B \ln r]^{1/2} \frac{1}{r^{\mu}} F(r/L), \tag{31}$$

where F is an unknown function. Since $\mu=0.5$ for $s=2$, we plot $C^2(r)r$ for fixed r/L as a function of $\ln L$. The result should be a straight line, with slope $BF^2(r/L)$. The results are shown in Fig. 7. For all the values of r/L shown, there is an upward curvature to the plots. This is presumably due to subleading corrections to the scaling form, since the leading

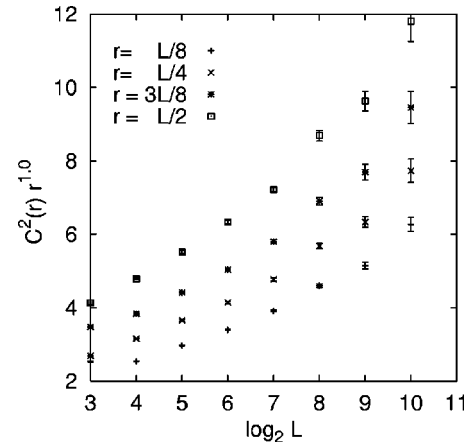

FIG. 7. Plot of $C^2(r)r$ for fixed r/L as a function of $\log_2 L$, for $s=2$. Four different values of r/L are shown. The vertical bars are the error bars. There is a noticeable odd-even effect for $r=L/8$ and $r=3L/8$ for $L=8$. For all the values of r/L, the plots curve slightly upward.

correction is large enough to change the effective μ in Eq. (31) from 0.5 to 0.4.

V. CONCLUSION

In this paper, we have proposed a generalization of the Gutzwiller wave function for spin $\frac{1}{2}$ chains that yields simple wave functions for spin chains with $s>\frac{1}{2}$. Remarkably, the spin spin correlation functions for these wave functions have the same power law decay as Wess Zumino Witten models with $k=2s$, in contrast to the generic expectation of $k=1$ for all half-integer spin and an exponential decay for integer spin. This result was obtained through numerical simulations for $s=1$, $\frac{3}{2}$, and 2, after mapping the model to a classical statistical mechanical model with long range interacting spin chains.

In summary, we have taken free fermionic wave functions and found a way of projecting them in a fashion that yields the WZW theory exponents, a possibility that has been presaged in Ref. 17. It remains to be seen if there is a systematic way of finding Hamiltonians for which the wave functions presented here are ground states.

[1] H.A. Bethe, Z. Phys. **71**, 205 (1931).
[2] F.D.M. Haldane, Phys. Lett. A **93**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).
[3] L. Takhtajan, Phys. Lett. A **90**, 479 (1982); J. Babudjian, Nucl. Phys. B **125**, 317 (1983).
[4] P. Kulish and F. Sklyanin, *Lecture Notes in Physics 151* (Springer, Berlin, 1982), p. 61; P. Kulish, N. Yu. Reshetikhin, and E. Sklyanin, Lett. Math. Phys. **5**, 393 (1981).
[5] I. Affleck, Phys. Rev. Lett. **55**, 1355 (1985); Nucl. Phys. B **265**, 409 (1986).
[6] I. Affleck, D. Gepner, H.J. Schulz, and T. Ziman, J. Phys. A **22**, 511 (1989).
[7] F.D.M. Haldane, Phys. Rev. Lett. **60**, 635 (1988).
[8] B.S. Shastry, Phys. Rev. Lett. **60**, 639 (1988).
[9] T.A. Kaplan, P. Horsch, and P. Fulde, Phys. Rev. Lett. **49**, 889 (1982); C. Gros, R. Joynt, and T.M. Rice, Phys. Rev. B **36**, 381 (1987); F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59**, 1472 (1987).
[10] B.S. Shastry, Phys. Rev. B **46**, 8263 (1992).
[11] D.P. Arovas, A. Auerbach, and F.D.M. Haldane, Phys. Rev. Lett. **60**, 531 (1988); S.M. Girvin and D.P. Arovas, Phys. Scr., T **T27**, 156 (1989).
[12] I. Affleck, T. Kennedy, E.H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987), Commun. Math. Phys. **115**, 477 (1988).
[13] O. Narayan and B.S. Shastry, J. Phys. A **32**, 1131 (1999).
[14] J.M. Radcliffe, J. Phys. A **4**, 313 (1971).
[15] B.S. Shastry, G.S. Agarwal, and I. Rama Rao, Pramana **11**, 85 (1978).
[16] F. Arecchi, E. Courtens, R. Gilmore, and H. Thomas, Phys. Rev. A **6**, 2211 (1972).
[17] A.O.Gogolin, A.A. Nersesyan, and A.M. Tsvelik, *Bosonization and Strongly Correlated Systems* (Cambridge University Press, Cambridge), 1998, Chap. 7, p. 56.