Majorana fermion representation for an antiferromagnetic spin-$\frac{1}{2}$ chain

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(Received 28 March 1996; revised manuscript received 29 May 1996)

We study the one-dimensional Heisenberg antiferromagnet with $s = \frac{1}{2}$ using a Majorana representation of the $s = \frac{1}{2}$ spins. A simple Hartree-Fock approximation of the resulting model gives a bilinear fermionic description of the model. This description is rotationally invariant and gives power-law correlations in the ''ground state'' in a natural fashion. The excitations are a two-parameter family of particles, which are spin-1 objects. These are contrasted to the ''spinon'' spectrum, and the technical aspects of the representation are discussed, including the problem of redundant states. [S0163-1829(97)01805-5]

I. INTRODUCTION

The study of various representations of spins in terms of bosonic or fermionic operators is an old and well-studied problem, reviewed nicely, for example, in Ref. 1. The need for exploring various representations has received a further impetus from the recent interest in the Heisenberg antiferromagnet, as a standard model in the resonating valence bond theories,[2] i.e., models where states with no long ranged Néel order play an important role. The Schwinger boson representation is of very general validity, i.e., for any s, but the Schwinger fermionic representation is only valid for $s = \frac{1}{2}$ and gives $s_i^\alpha = \frac{1}{2}\Sigma_{\sigma,\sigma'} c_{i\sigma}^\dagger \tau^\alpha c_{i,\sigma'}$, with the constraint $\Sigma_\sigma c_\sigma^\dagger c_\sigma = 1$.[3,4] The constraint is not very easy to deal with, except in an averaged sense. Hence one may look for unconstrained representations. For $s = \frac{1}{2}$ such unconstrained representations can be found. The so-called ''drone fermion'' representation[5,6,1] is one of the possibilities, where we write $s_i^+ = a_i^\dagger \phi_i$, $s_i^- = \phi_i a_i$, and $s_i^z = a_i^\dagger a_i - \frac{1}{2}$, where the a's are canonical anticommuting variables, and ϕ_i is a *real* fermion with $\phi^\dagger = \phi$ and $\phi^2 = 1$. Thus ϕ is a ''drone'' whose only 'job' is to make spins at different sites commute, rather than anticommute. In single-site problems like the Kondo problem, these are useful.[6] However, this representation violates rotation invariance, since our choice of the z axis was arbitrary. A fully rotation invariant scheme does exist, and can, for example, be derived from the above, by simply rewriting the complex fermion a in terms of its two real components as $a \propto \phi_x + i\phi_y$. This leads to a representation with three Majorana fields, and is studied in this paper, in the context of the one-dimensional Heisenberg model.

The plan of this paper is as follows. In Sec. II, we discuss the Majorana representation and the need for enlarging the Hilbert space of states in order to obtain a representation of the Majorana algebra. We introduce the spin-$\frac{1}{2}$ antiferromagnetic chain and its low-lying excitations in Sec. III. In Sec. IV, we use the Majorana representation to study the chain within a rotationally invariant Hartree-Fock (HF) approximation. Since the HF approximation is not unique in the general case, we require that the susceptibility calculated by two methods, namely, from the energy change and from the fluctuation spectrum, should agree. This requirement, interestingly, rules out several possibilities, and leads to a particular scheme which is implemented. We obtain a spectrum of low-lying excitations which bears a strong resemblance to the one discussed in Sec. III.

We also discuss the spin of the Majorana fermion. In Sec. V, we compute the dynamic structure function and susceptibility, at both zero and finite temperatures, and contrast these with previously known results. In Sec. VI, we study the response of the model to uniform and staggered magnetic fields. We end with some concluding remarks in Sec. VII.

II. MAJORANA REPRESENTATION

At each site n, we can write the spin operators $\vec{S}_n = \vec{\sigma}_n/2$ in terms of three Majorana operators $\vec{\phi}_n$ as[7–9]

$$\sigma_n^x = -i\phi_n^y \phi_n^z, \quad \sigma_n^y = -i\phi_n^z \phi_n^x,$$

and

$$\sigma_n^z = -i\phi_n^x \phi_n^y. \tag{1}$$

(We set Planck's constant equal to 1.) The operators ϕ_n^a (with $a = x,y,z$) are Hermitian and satisfy the anticommutation relations

$$\{\phi_m^a, \phi_n^b\} = 2\delta_{mn}\delta_{ab}. \tag{2}$$

It is interesting to note that the relation $\vec{S}_n^2 = 3/4$ automatically follows from Eqs. (1) and (2); one does not have to impose any additional constraints at each site unlike the Schwinger representation.[3] There is a local Z_2 gauge invariance since changing the sign of $\vec{\phi}_n$ does not affect $\vec{S}_n$. [The Schwinger representation has a local U(1) gauge invariance].

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For N sites with a spin-$\frac{1}{2}$ object at each site, the Hilbert space clearly has a dimension 2^N. We now ask what is the minimum possible dimension which will allow a representation of the form given in Eqs. (1) and (2)? The answer is $2^{N+[N/2]}$, where $[N/2]$ denotes the largest integer less than or equal to $N/2$. This follows from the observation that a representation for Eqs. (1) and (2) is given by

$$\phi_n^a = \sigma_n^a \psi_n ,$$

where

$$[\sigma_m^a , \psi_n] = 0,$$

and

$$\{\psi_m , \psi_n\} = 2\,\delta_{mn} . \tag{3}$$

The minimum dimension required for a matrix representation of the spinless anticommuting operators ψ_n is $2^{[N/2]}$.[9] Thus the Majorana representation of spin-$\frac{1}{2}$ objects requires us to enlarge the space of states; the complete Hilbert space of states is given by a direct product of a ''physical'' space and an ''unphysical'' one. Now suppose that the Hamiltonian is purely a function of the physical operators $\vec{S}_n$; it therefore only acts on the physical states. Then the unphysical part of the Hilbert space simply factorizes out; hence each value of the energy will have a degeneracy of $2^{[N/2]}$.

As an explicit example, consider the case $N=2$. The Majorana Hilbert space is eight-dimensional, where the extra factor of 2 arises from the unphysical space. We can denote the eight states as $\uparrow\uparrow\uparrow$, $\uparrow\uparrow\downarrow$, etc. The physical operators $\vec{S}_1$ and $\vec{S}_2$ only act on the first and second symbols, respectively. The third symbol, which may be $\uparrow$ or $\downarrow$, denotes the unphysical space. A Hamiltonian of the form $\vec{S}_1 \cdot \vec{S}_2$ only acts on the first two symbols; hence the energy levels will be precisely the ones of a two-site antiferromagnet, but with an additional degeneracy of 2 due to the third symbol. On the other hand, the Majorana operators can be written in the direct product form

$$\vec{\phi}_1 = \vec{\sigma} \otimes 1 \otimes \sigma^x$$

and

$$\vec{\phi}_2 = 1 \otimes \vec{\sigma} \otimes \sigma^y . \tag{4}$$

Hence they act on the third symbol and can therefore mix up physical and unphysical states.

One might worry that thermodynamic quantities like the entropy will get a spurious contribution proportional to N due to the unphysical degeneracy of $2^{[N/2]}$. On the other hand, when we make approximations like the HF decomposition discussed later, the physical and unphysical states get mixed up in an essential way. This completely changes the energy degeneracy; in particular, the HF ground state is actually unique as we will see.

We can think of ϕ_n^a as the fundamental field in our theory. Both σ_n^a and ψ_n can be written in terms of ϕ_n^a, as can be seen from Eq. (1) and $\psi_n = -i\,\phi_n^x \phi_n^y \phi_n^z$, respectively.

III. ANTIFERROMAGNETIC SPIN-$\frac{1}{2}$ CHAIN

We will now begin our analysis of a Heisenberg antiferromagnetic chain. The Hamiltonian is

$$H = J \sum_n \vec{S}_n \cdot \vec{S}_{n+1} , \tag{5}$$

where the exchange constant $J>0$. We use periodic boundary conditions $\vec{S}_{N+1} = \vec{S}_1$. (We set the lattice spacing $a=1$.) The spectrum of Eq. (5) is exactly solvable by the Bethe ansatz; in particular, the ground state energy is given by $E_0 = (-\ln 2 + 1/4)NJ = -0.4431NJ$. The lowest excitations are known to be fourfold degenerate consisting of a triplet $(S=1)$ and a singlet $(S=0)$.[11] The excitation spectrum is described by a two-parameter continuum in the (q,ω) space, where $-\pi < q \leqslant \pi$. The lower boundary of the continuum is described by the des Cloiseaux-Pearson relation[10]

$$\omega_l(q) = \frac{\pi J}{2} |\sin q| , \tag{6}$$

whereas the upper boundary is given by

$$\omega_u(q) = \pi J \left| \sin \frac{q}{2} \right| . \tag{7}$$

We can understand this continuum by thinking of these excitations as being made up of two spin-$\frac{1}{2}$ objects (''spinons'') with the dispersion[11]

$$\omega(q) = \frac{\pi J}{2} \sin q , \tag{8}$$

where $0<q<\pi$. A triplet (or a singlet) excitation with momentum q is made up of two spinons with momenta q_1 and q_2, such that $0<q_1 \leqslant q_2 < \pi$, $q=q_1+q_2$ if $0<q\leqslant\pi$, and $q=q_1+q_2-2\pi$ if $-\pi<q<0$; further, $\omega(q)=\omega(q_1)+\omega(q_2)$. The two-parameter continuum arises because q_1 can vary from 0 to $q/2$ if $0<q<\pi$, and from $\pi+q$ to $\pi+q/2$ if $-\pi<q<0$.

IV. HARTREE-FOCK TREATMENT, GROUND STATE, AND EXCITATIONS

We will now study this system using the Majorana representation. We write Eq. (5) in terms of Majorana operators to get a quartic expression, and then perform a Hartree-Fock (HF) decomposition. Thus we write

$$H = -\frac{J}{4}\sum_n \left[\phi_n^x \phi_n^y \phi_{n+1}^x \phi_{n+1}^y + \text{ cycl. perm. } (x,y,z)\right]$$

$$\simeq \frac{J}{4}\sum_n \left[\phi_n^x \phi_{n+1}^x \langle \phi_n^y \phi_{n+1}^y \rangle + \langle \phi_n^x \phi_{n+1}^x \rangle \phi_n^y \phi_{n+1}^y - \langle \phi_n^x \phi_{n+1}^x \rangle \langle \phi_n^y \phi_{n+1}^y \rangle + \text{ cycl. perm. } (x,y,z)\right]. \tag{9}$$

In principle, the HF can be done in three different ways; however, rotational invariance implies that only one kind of bilinear can have a nonzero expectation value in the ground state, namely,

$$g = -i\langle \phi_n^a \phi_{n+1}^a \rangle, \tag{10}$$

where g has the same value for $a = x,y,z$; we also assume it to be translation invariant. The value of g will be determined self-consistently. We now have to diagonalize the quadratic Hamiltonian

$$H = \frac{iJg}{2}\sum_{a,n} \phi_n^a \phi_{n+1}^a + \frac{3}{4}NJg^2. \tag{11}$$

Since ϕ_n^a is Hermitian, its Fourier expansion can be defined as

$$\phi_n^a = \sqrt{\frac{2}{N}}\sum_{0<q<\pi} [b_{aq}^\dagger e^{iqn} + b_{aq} e^{-iqn}], \tag{12}$$

where

$$\{b_{aq}, b_{bq'}^\dagger\} = \delta_{ab}\delta_{qq'}. \tag{13}$$

A similar half-zone definition of the Fourier transforms is possible in higher dimensions as well; for example, on the square lattice, we could restrict the sum to $q_x > 0$. We will work with *antiperiodic* boundary conditions for ϕ_n^a and *even* values of N in order to eliminate modes with q equal to 0 and π. This simplifies the calculation because the momenta q and $-q$ are then distinct points in the Brillouin zone extending from $-\pi$ to π. In Eq. (12), $q = 2\pi(p - 1/2)/N$, with $p = 1,2,\ldots,N/2$. In the limit $N \to \infty$, we get

$$H = \sum_a \sum_{0<q<\pi} \omega(q) b_{aq}^\dagger b_{aq} + 3NJ\left(\frac{g^2}{4} - \frac{g}{\pi}\right), \tag{14}$$

where the Majorana fermions have the dispersion

$$\omega(q) = c \sin q, \tag{15}$$

with $c = 2gJ$. The HF ground state $|0\rangle$ is therefore the state annihilated by all the b_{aq}. Note that it is unique unlike the *exact* ground state, which has a degeneracy of $2^{N/2}$ within the Majorana formalism. It is curious that the HF approximation gives a unique ground state which agrees with the degeneracy we would have obtained *without* the Majorana formalism.

We now calculate Eq. (10) in the HF ground state and obtain

$$g = \frac{2}{\pi}. \tag{16}$$

The HF ground state energy is therefore

$$E_{0\,\mathrm{HF}} = -\frac{3}{\pi^2}NJ = -0.3040NJ. \tag{17}$$

This is greater than the exact value mentioned above; indeed, one can show that *any* HF decomposition must give an estimate for the ground state energy which is bounded below by the exact value E_0. The argument goes as follows. In Sec. II, we have shown that the exact ground state energy within the Majorana formalism is equal to the exact ground state E_0 without the Majorana formalism, since the Hamiltonian H only acts on physical states. Let us therefore prove the upper bound result in the Majorana Hilbert space which includes both physical and unphysical states. Now the HF calculation is equivalent to self-consistently finding an ansatz ground state $|0\rangle$ and caclulating the expectation value of H in that. (One can show that $|0\rangle$ is an eigenstate of the Majorana fermion number operator. Hence an expectation value of the form $\langle ABCD\rangle$ is indeed given by the HF decomposition $\langle AB\rangle\langle CD\rangle - \langle AC\rangle\langle BD\rangle + \langle AD\rangle\langle BC\rangle$, if the operators A, B, C, and D are all fermionic.) By the variational argument, the expectation value of H in any state is bounded below by E_0.

The ''spinon'' spectrum has the same form as in Eq. (8) but has a different coefficient $c_{\mathrm{exact}} = \pi J/2$, whereas we find $c = 4J/\pi$ from Eq. (16). Note that the self-consistent equation Eq. (10) also leads to Eq. (16), since we have

$$-i\sum_n \phi_n^x \phi_{n+1}^x = \frac{2N}{\pi} - 4\sum_{q>0} \sin q\, b_{xq}^\dagger b_{xq}. \tag{18}$$

The ground state is a singlet since it is annihilated by the total spin $\vec{S}_{\mathrm{tot}} = \Sigma_n \vec{S}_n$, for instance, by

$$S_{\mathrm{tot}}^z = -i\sum_{0<q<\pi} (b_{xq}^\dagger b_{yq} - b_{yq}^\dagger b_{xq}). \tag{19}$$

We now ask what is the spin of a Majorana fermion? From the commutation relations between $\vec{S}$ and $b_{aq}^\dagger$, we find that the one-fermion state $b_{aq}^\dagger|0\rangle$ has $S = 1$. More specifically, the states $(b_{xq}^\dagger + ib_{yq}^\dagger)|0\rangle$, $b_{zq}^\dagger|0\rangle$, and $(b_{xq}^\dagger - ib_{yq}^\dagger)|0\rangle$ have $S^z = 1$, 0, and -1, respectively.

A two-fermion state can therefore have $S = 0$, 1, or 2 in general. However the state created by $S_q^z = \Sigma_n S_n^z e^{-iqn}$, where $0 < q < \pi$, has the form

$$S_q^z|0\rangle = -i\sum_{0<k<q/2} (b_{xk}^\dagger b_{y,q-k}^\dagger - b_{yk}^\dagger b_{x,q-k}^\dagger)|0\rangle, \tag{20}$$

and can be shown to have $S=1$. We have thus derived the two-parameter continuum of triplet excitations in Eqs. (6) and (7), with a prefactor $4/\pi$ instead of $\pi/2$.

Finally, we can compute the equal-time two-spin correlation function

$$G_n \equiv \langle 0|\vec{S}_0\cdot\vec{S}_n|0\rangle = \begin{cases} \frac{3}{4} & \text{for } n=0, \\ -\frac{3}{2\pi^2 n^2}[1-(-1)^n] & \text{for } n\neq 0. \end{cases} \tag{21}$$

This does not agree with the correct asymptotic behavior of G_n which is known to oscillate as $(-1)^n/n$. In particular, the HF static structure function $S(q)=\Sigma_n G_n e^{-iqn}$ does not diverge as $q\to\pi$ in contrast to the correct $S(q)$ which has a logarithmic divergence at π. Note that $\Sigma_n G_n=0$, as expected for a singlet ground state. It is interesting to observe that the Schwinger fermion representation yields a correlation function which only differs from Eq. (21) by a numerical factor (see the first reference in Ref. 3).

This Hartree-Fock state is readily generalized to finite temperatures, since we simply need to put in thermal population factors for the occupations of the fermions

$$\langle b^\dagger_{aq} b_{aq}\rangle = \frac{1}{1+\exp(\beta c\sin q)}. \tag{22}$$

Hence the self-consistency condition Eq. (10) together with Eqs. (18) and (22) gives us

$$g=\frac{2}{\pi}-\frac{4}{N}\sum_{q>0}\frac{\sin q}{1+\exp(\beta c \sin q)}. \tag{23}$$

It is easy to see that as $T\to\infty$ we have $g\to 0$, and as $T\to 0$ we have $g\to(2/\pi)(1-\pi^2 k_B^2 T^2/6c^2)$, i.e., a power-law correction to the zero-temperature ''bandwidth'' g.

The HF ground state discussed above is, unfortunately, not the one with the lowest energy. If we allow a dimerized expectation value g_n in Eq. (10), where g_n can alternate in strength from bond to bond, we find that the lowest energy is attained for the fully dimerized state in which $g_n=1$ for n even and 0 for n odd (or vice versa). This corresponds to a dimerized ground state with an energy

$$E_{0\,\text{dim}}=-\frac{3}{8}NJ, \tag{24}$$

which is substantially lower than the earlier HF value. There is a gap equal to J above the dimerized ground state. [This ground state is, of course, exact for the case $N=2$ (Ref. 12).] The reader may wonder why we are ignoring the dimerized HF state in the rest of this paper, even though it has the lowest HF energy. The reason is that we know by other methods, both analytical and numerical, that the correct ground state of the spin-$\frac{1}{2}$ chain is translation invariant and that there is no gap above it. The HF method is, after all, only an approximation, and different approximations can certainly give different results. We should therefore pick the HF which agrees qualitatively with other methods; the ground state energy is not necessarily the best criterion for choosing one HF over another. Having chosen a particular HF on the basis of certain features, we of course have to check whether it reproduces other features equally well. We will see in Secs. V and VI that the translation invariant HF yields reasonable results for the structure functions and susceptibilites also.

V. DYNAMIC STRUCTURE FUNCTION AND SUSCEPTIBILITY

We recall the definition of the dynamical susceptibility

$$\chi^{zz}(Q,t)=i\theta(t)\langle[S^z_{-Q}(t),S^z_Q]\rangle, \tag{25}$$

$$\chi^{zz}(Q,\omega)=\int_{-\infty}^{+\infty}dt\,\chi^{zz}(Q,t)\exp(i\omega t) \tag{26}$$

$$=\sum_{\mu,\nu}\frac{\exp(-\beta\epsilon_\nu)-\exp(-\beta\epsilon_\mu)}{\epsilon_\mu-\epsilon_\nu+\omega+i0^+}\times\langle\mu|S^z_{-Q}|\nu\rangle\langle\nu|S^z_Q|\mu\rangle. \tag{27}$$

The Zeeman coupling of a spin to a magnetic field is given by $g_l\mu_B S^z B$, where g_l and μ_B denote the Lande g factor and the Bohr magneton, respectively. The physical response function (i.e., $g_l\mu_B\langle S^z\rangle$) is $\chi=g_l^2\mu_B^2\chi^{zz}(Q,\omega)$. In the static limit $\omega=0$, we have the usual thermodynamic argument for determining the susceptibility. If we perturb the system via the coupling $H=H_0-g_l\mu_B B\Sigma_n\cos(Qn)S^z_n$, then the change in the free energy is $\delta F=-g_l^2\mu_B^2 B^2\chi^{zz}(Q,0)\theta_Q$, where $\theta_Q=1/4$ if $Q\neq 0,\pi$, and $\theta_0=1/2=\theta_\pi$. (This factor of θ arises because for a finite Q we drop two of the four terms in second-order perturbation theory using momentum conservation; this neglect is disallowed exactly at $Q=0,\pi$.) Also recall that the static correlation function is given by

$$\langle S^z_{-Q}S^z_Q\rangle=\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\frac{\text{Im}\chi^{zz}(Q,\omega)}{1-\exp(-\beta\omega)}. \tag{28}$$

We will now compute the response functions in the HF approximation. We begin by expressing, for $0<Q<\pi$, the operator S^z_Q in terms of the Majorana fields in the Heisenberg picture:

$$\begin{aligned} S^z_Q(t)=&-i\sum_{0<q<Q}\alpha(q,Q-q)b^\dagger_{xq}b^\dagger_{y,Q-q}\exp i(\omega_q+\omega_{Q-q})t \\ &-i\sum_{\pi-Q<q<\pi}\alpha(q,2\pi-Q-q)b_{xq}b_{y,2\pi-Q-q} \\ &\times\exp -i(\omega_q+\omega_{2\pi-Q-q})t-i\sum_{Q<q<\pi}\gamma(q,q-Q) \\ &\times[b^\dagger_{xq}b_{y,q-Q}-b^\dagger_{yq}b_{x,q-Q}]\exp i(\omega_q-\omega_{q-Q})t. \end{aligned} \tag{29}$$

In this equation we have introduced two real phenomenological functions $\alpha(a,b)=\alpha(b,a)=\alpha(\pi-a,\pi-b)$ and $\gamma(a,b)$ which are, strictly speaking, equal to unity from the Majorana definition of the spins. These are introduced in order to facilitate the comparison of our structure function with a phenomenological function proposed in Ref. 13. The essential point is that we have assumed that the time evolution is given by the bilinear in fermions, our Eq. (14). The representation for S^z_{-Q} is obtained by taking Hermitian conjugates. Note that S^z_Q or S^z_{-Q} acting on the ground state generates two spinons. We insert it in Eq. (26), carry out the contraction of the fermions by Wick's theorem, and use Eq. (22) in the form $n_q=\langle b^\dagger_{q,\alpha}b_{q,\alpha}\rangle$ and $\overline{n_q}=1-n_q$ to find

$$\chi^{zz}(Q,\omega)=\sum_{0<q<Q}\alpha^2(q,Q-q)\,\frac{\overline{n_q n_{Q-q}}-n_q n_{Q-q}}{\omega_q+\omega_{Q-q}-\omega-i0^+}+\sum_{0<q<Q}\alpha^2(q,Q-q)\,\frac{\overline{n_q n_{Q-q}}-n_q n_{Q-q}}{\omega_q+\omega_{Q-q}+\omega+i0^+}+2\sum_{Q<q<\pi}\gamma^2(q,q-Q)\,\frac{n_{q-Q}\overline{n_q}-\overline{n_{q-Q}}n_q}{\omega_q-\omega_{q-Q}-\omega-i0^+}. \tag{30}$$

This is seen to be an even function of ω by using $q\to\pi+Q-q$ in the last term. Using Eq. (28), we deduce that

$$G^{zz}(Q)\equiv\langle S^z_{-Q}S^z_Q\rangle=\sum_{0<q<Q}\alpha^2(q,Q-q)[\overline{n_q n_{Q-q}}+n_q n_{Q-q}]+2\sum_{Q<q<\pi}\gamma^2(q,q-Q)n_{q-Q}\overline{n_q}. \tag{31}$$

Let us note that at zero temperature, if we set $\alpha=\gamma=1$, we get $G^{zz}(Q)=N|Q|/2\pi$ and hence the correlation function quoted in Eq. (21). At the other extreme limit $T\to\infty$, we replace $n=\overline{n}=1/2$ and find $G^{zz}(Q)=N/4$. At *any* temperature, the relation $n_q+\overline{n_q}=1$ allows us to show that the sum rule $\langle S^z_n S^z_n\rangle=1/4$ is satisfied.

At zero temperature, we have the static susceptibility

$$\chi^{zz}(Q,0)=2\sum_{0<q<Q}\frac{\alpha^2(q,Q-q)}{\omega_q+\omega_{Q-q}} \tag{32}$$

which, in the standard situation $\alpha=1$, can be evaluated in the closed form

$$\chi^{zz}(Q,0)=\frac{N}{\pi c\sin(Q/2)}\ln\left(\frac{\cos(\pi-Q)/4}{\cos(\pi+Q)/4}\right). \tag{33}$$

The uniform value is

$$\chi^{zz}(0,0)=\frac{N}{\pi c}=\frac{N}{4J}. \tag{34}$$

The neutron scattering function which is of particular interest is found at zero temperature as

$$\mathrm{Im}\chi^{zz}(Q,\omega)=\pi\sum_{0<q<Q}\alpha^2(q,Q-q)\,\delta(\omega_q+\omega_{Q-q}-\omega) \tag{35}$$

for $\omega>0$. We can evaluate it in terms of the dimensionless energies $u\equiv\omega/c$, $u_>\equiv 2\sin(Q/2)$ and $u_<\equiv\sin Q$, as

$$\mathrm{Im}\chi^{zz}(Q,\omega)=\frac{N}{c}\,\frac{\alpha^2(q^*,Q-q^*)}{|\cos(q^*)-\cos(Q-q^*)|}\times\theta(u_>-u)\,\theta(u-u_<), \tag{36}$$

where q^* is the solution of $\sin q^*+\sin(Q-q^*)=u$ which equals $Q/2$ at $u=u_>$. With this we find

$$\sin q^*=\frac{1}{2}[u-\cot(Q/2)\sqrt{u_>^2-u^2}],$$

$$\cos q^*=\frac{1}{2}[u\cot(Q/2)+\sqrt{u_>^2-u^2}]. \tag{37}$$

This implies that $|\cos(q^*)-\cos(Q-q^*)|=\sqrt{u_>^2-u^2}$, and

$$\mathrm{Im}\chi^{zz}(Q,\omega)=\frac{N}{c}\,\frac{\alpha^2(q^*,Q-q^*)}{\sqrt{u_>^2-u^2}}\theta(u_>-u)\,\theta(u-u_<). \tag{38}$$

This susceptibility is very similar to that proposed in Ref. 13 phenomenologically, and also found for the long ranged spin-$\frac{1}{2}$ chain[14,15] in Ref. 16, with one important difference. The spectral weight here is dominatd by the upper threshold of the two-parameter continuum $u_>$, whereas the weight is peaked at the lower threshold $u_<$ in Ref. 13. It is straightforward to see that if we choose

$$\alpha^2(q,Q-q)\equiv\nu\frac{|\sin(Q/2-q)|}{\sqrt{\sin q}\sqrt{\sin(Q-q)}}, \tag{39}$$

then on using Eq. (37), the weight is shifted to the bottom, and we get

$$\mathrm{Im}\chi^{zz}(Q,\omega)=\frac{N\nu}{c}\,\frac{1}{\sqrt{u^2-u_<^2}}\,\theta(u_>-u)\,\theta(u-u_<). \tag{40}$$

With this choice, the static correlation function can be evaluated from Eq. (28). We find

$$G^{zz}(Q)=\frac{N\nu}{\pi}\ln\left(\frac{1+\sin(Q/2)}{\cos(Q/2)}\right), \tag{41}$$

leading to the asymptotic behavior $\sim(-1)^n/n$ at long distances. Indeed one can use the two parameters c and ν in Eqs. (40) and (41) together with the various sum rules known, in order to obtain very realistic structure functions which mimic the behavior of the nearest neighbor Heisenberg antiferromagnet. At finite temperatures, we find from Eq. (31) in the usual case of $\alpha=\gamma=1$

$$\langle S^z_n S^z_0\rangle=\frac{1}{4}\,\delta_{n,0}-\frac{1}{16}\left[f_n\left(\frac{\beta c}{2}\right)\right]^2, \tag{42}$$

with

$$f_n\left(\frac{\beta c}{2}\right)=\frac{2}{\pi}\int_0^\pi dx\,\sin(nx)\tanh\left(\frac{\beta c}{2}\sin x\right), \tag{43}$$

leading to an exponentially decaying correlation function with a correlation length $\xi\sim 1/T$ for $T\to 0$. The function f_n vanishes for even n in contrast to one's usual expectation. In the presence of the phenomenological α, one must necessarily cut off the linear divergence of α at $Q=\pi$ and $q\sim 0,\pi$. A temperature dependent cutoff, such as

$$\alpha^2(a,b)=(|\sin(a-b)/2| +(\text{const})^2T)/[\sqrt{\sin(a)+(\text{const})T} \times\sqrt{\sin(b)+(\text{const})T}]$$

interpolates nicely between the zero-temperature limit and the high temperature limit, and again gives a correlation length $\sim 1/T$.

VI. MAGNETIC FIELDS

We will now discuss the HF ground state of the spin chain in the presence of uniform and staggered magnetic fields, and calculate the two susceptibilities.

A. Uniform magnetic field

For a uniform magnetic field $B\hat{z}$, we add a term $-g_l\mu_B B\Sigma_n S_n^z$ to the Hamiltonian (5). Since this term commutes with Eq. (5), we can use the same HF decomposition as in Eq. (10) with $g=2/\pi$. Since the extra term in the Hamiltonian is quadratic in the Majorana operators, we only have to perform a rediagonalization of Eq. (11). We find that modes with $S^z=\pm 1$ have an energy

$$\omega_\pm(q)=\frac{4J}{\pi}\sin q\mp g_l\mu_B B, \tag{44}$$

while the energy of the $S^z=0$ modes remain unchanged. For $B>0$, let us define a momentum q_0 such that

$$q_0=\sin^{-1}\left(\frac{\pi g_l\mu_B B}{4J}\right), \tag{45}$$

and $0<q_0<\pi/2$. (Such a q_0 exists only if the magnetic field is less than a critical value $B_c=4J/\pi g_l\mu_B$). Then the modes with $S^z=1$ and momenta lying in the range $0<q<q_0$ and $\pi-q_0<q<\pi$ have negative energy, and the ground state of the system is one in which those modes are occupied. The change in the ground state energy is therefore given by a sum over all the occupied modes q,

$$\Delta E_{0\,\mathrm{HF}}=\sum_q\left(\frac{4J}{\pi}\sin q-g_l\mu_B B\right) =\frac{4NJ}{\pi^2}(1-\cos q_0)-\frac{Ng_l\mu_B B}{\pi}q_0. \tag{46}$$

The expectation value of S^z in the ground state is obtained either by counting the number of occupied modes, or by differentiating Eq. (46) with respect to $g_l\mu_B B$. Thus

$$\langle S^z\rangle=\frac{Nq_0}{\pi}=\frac{N}{\pi}\sin^{-1}\left(\frac{\pi g_l\mu_B B}{4J}\right). \tag{47}$$

Finally, the (uniform) susceptibility is given by

$$\chi=\frac{1}{g_l\mu_B}\left(\frac{\partial\langle S^z\rangle}{\partial B}\right)_{B=0}=\frac{N}{4J}. \tag{48}$$

This agrees with the result in the previous section. For a strong magnetic field $B>B_c$, the ground state is fully polarized with $S^z=N/2$. These results are to be compared with the exact results for the susceptibility $\chi=N/\pi^2J$, and the critical field $B_c=2J/g_l\mu_B$.[13]

Since S_n^z has a nonzero expectation value in the ground state, the above calculation is not entirely self-consistent, i.e., one should also allow HF decompositions of the form

$$\langle\phi_n^x\phi_n^y\rangle=if_0$$

and

$$\langle\phi_n^x\phi_{n\pm1}^y\rangle=if_{\pm1}. \tag{49}$$

Further, the expectation values

$$\langle\phi_n^x\phi_{n+1}^x\rangle=\langle\phi_n^y\phi_{n+1}^y\rangle=ig_T$$

and

$$\langle\phi_n^z\phi_{n+1}^z\rangle=ig_L \tag{50}$$

may be unequal since the magnetic field breaks rotational invariance. On doing this more general HF calculation, we find that although the ground state remains the same qualitatively (i.e., a number of $S^z=1$ modes have to be filled in the regions $0<q<q_0$ and $\pi-q_0<q<\pi$), various numbers change. For instance, q_0 is now given by

$$q_0+\sin q_0(1+\cos q_0)=\frac{\pi g_l\mu_B B}{2J}. \tag{51}$$

The HF parameters are

$$g_T=\frac{2}{\pi}\cos q_0,\quad g_L=\frac{2}{\pi},$$

$$f_0=\frac{2q_0}{\pi},\quad f_{\pm1}=0. \tag{52}$$

Since the magnetization is equal to Nq_0/π, the susceptibilty is $\chi=N/6J$. [The critical field for complete polarization is $B_c=J(1+2/\pi)/g_l\mu_B$.] We therefore have the curious result that a completely self-consistent HF calculation does not agree with linear response theory for small fields.

B. Staggered magnetic field

We now study the situation with a staggered magnetic field. We add a term $-g_l\mu_B B\Sigma_n(-1)^n S_n^z$ to the Hamiltonian and perform a HF decomposition. As in the uniform case, we will assume that $g_T=g_L=2/\pi$ and $f_0=f_{\pm1}=0$ in Eqs. (49) and (50) even though this is not completely self-consistent. We then find that the dispersion of the longitudinal modes remain the same as before while those of the transverse modes change. To be explicit,

$$\omega_L(q)=\frac{4J}{\pi}\sin q$$

and

$$\omega_T(q)=\left(\frac{16J^2}{\pi^2}\sin^2 q+g_l^2\mu_B^2B^2\right)^{1/2}. \quad (53)$$

Further, the change in the ground state energy is

$$\Delta E_{0\text{HF}}=\sum_{0<q<\pi}\left(\frac{4J}{\pi}\sin q-\omega_T(q)\right). \quad (54)$$

On differentiating this with respect to $g_l\mu_B B$, we find the staggered magnetization to be

$$\left\langle\sum_n (-1)^n S_n^z\right\rangle=Ng_l\mu_B B\int_0^{2\pi}\frac{dq}{2\pi}\frac{1}{\omega_T(q)}. \quad (55)$$

For small fields, this goes as $(Ng_l\mu_B B/4J)\ln(J/g_l\mu_B B)$ which implies that the staggered susceptibility is divergent. This is the correct result. For large fields, the staggered magnetization approaches $N/2$ as it should.

VII. DISCUSSION

To summarize, we have used a Majorana fermion representation to study a nearest neighbor isotropic antiferromagnetic spin-$\frac{1}{2}$ chain. Within a translation invariant Hartree-Fock approximation, we have found the spectrum of low-lying excitations, the two-spin correlation function, the structure function, and the magnetic susceptibilities. All of these agree qualitatively with the results found earlier by a variety of other methods. The agreement can be made quantitative if we introduce some phenomenological functions within the Majorana formalism.

It is somewhat surprising that a fully dimerized Hartree-Fock approximation leads to a ground state with a lower energy. One way of stabilizing the translation invariant ground state with respect to the dimerized one is to apply an uniform magnetic field with a strength $B>0.5829B_c=0.7422J/g_l\mu_B$. Such a magnetic field lowers the energy of the translation invariant ground state below $-3NJ/8$, and does not change the energy of the dimerized ground state, for $B<J/g_l\mu_B$, due to the finite gap to spin excitations.

It would be interesting to go beyond our Hartree-Fock treatment and study the effects of fluctuations. Besides producing more accurate numbers for various quantities such as the spin wave velocity, such a study could also lead to a more detailed understanding of the ''spinons'' in a spin-$\frac{1}{2}$ chain in terms of Majorana fermions.

It may be instructive to examine models with anisotropy, frustration, and higher dimensionality using the Majorana representation, and to compare with known results. Amongst other things, this would help to determine the range of validity of this way of studying spin-$\frac{1}{2}$ systems.

We have briefly examined the ferromagnetic case in which the exchange constant in Eq. (5) is *negative*. We perform a nonrotation invariant Hartree-Fock decomposition by allowing $\sigma_n^z=-i\phi_n^x\phi_n^y$ to take an expectation value. We then obtain the correct ground state energy $E_0=NJ/4$, with the total $S^z=\pm N/2$. However, we get the wrong dispersion relation, including a gap, for the low-energy excitations. Thus the Majorana Hartree-Fock approximation is not a good starting point for studying the spin-$\frac{1}{2}$ ferromagnet.

ACKNOWLEDGMENTS

B.S.S. would like to thank several colleagues who have encouraged him to publish Ref. 7, particularly P. W. Anderson, G. Baskaran, and R. Shankar, which represented a preliminary version of this work. This work was supported in part by the National Science Foundation under Grant No. PHY94-07194.

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