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ABSTRACT

The ground state of closed Heisenberg spin chains with an odd number of sites has a chiral degeneracy, in addition to a two-fold Kramers degeneracy. A non-zero chirality implies that the spins are not coplanar, and is a measure of handedness. The chirality operator, which can be treated as a spin-1/2 operator, is explicitly constructed in terms of the spin operators, and is given as commutator of permutation operators.

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In tl is report, we investigate the chirality operator for Heisenberg spin chains. Usually the chirality operator is given in terms of fermion operators defined[1] through $\vec{s}_i \equiv c^\dagger_{i\alpha}\vec{\sigma}_{\alpha\beta}c_{i\beta}$, and the fermion hopping operator $T_{ij} = \sum_\alpha c^\dagger_{i\alpha}c_{j\alpha}$. The chirality operator is given as the imaginary part of difference of products of T operators along the two closed loops on a closed chain. Unscrambling the fermion operator to express the chirality operator in terms of the original spin operator can be tedious in general, though the answer for the case of three spins turns out to be very simple, a box product of the three spins $\vec{s}_1.\vec{s}_2 \times \vec{s}_3$. Below we give an explicit construction of the chirality operator in terms of the spin operators directly. We treat the chirality as a spin-1/2 operator $\vec{\chi}$, whose z-component is the usual chirality operator discussed above. The construction starts with defining the chiral-spin raising operator χ^+ and its hermitian conjugate, and χ^z is given by the commutator $2\chi^z = [\chi^+, \chi^-]$, from the standard spin-1/2 algebra. The the chiral raising and lowering operators are related to permutation operators (permutation operators naturally arise as the chirality can be changed by a permutation of the labels), which can be expressed explicitly in terms of the original spin operators.

The Heisenberg Hamiltonian is given by

$$H = \sum_i \vec{s}_i.\vec{s}_{i+1}$$

where the sum is over N sites of a closed chain. We consider the case of an $N = 3$ as it is the simplest case, and generalize for any odd N later. The ground state for an odd-numbered chain belongs to the sector with the total spin $S = 1/2, S^Z = \pm 1/2$r, implying a two-fold Kramers degeneracy. However, each of the sectors with $S^z = \pm 1/2$ is further two-fold degenerate. This extra degeneracy is due to chirality. The two chiral states in $S^z = 1/2$ sector can be written in basis as

$$\phi_\pm = \sum_l e^{\pm ik(l-1)}|l>$$

where $k = 2\pi/3$ and $|l >= s_l^-| \uparrow\uparrow\uparrow>$. The two ground states in $S^z = -1/2$ sector are obtained by operating on the states above with the total spin lowering operator. The two chiral states have spin currents going in two different directions. For $N \neq 3$, the spin current corresponds to the motion of the center of mass of the down spins. We refer to these two states as having chirality by defining $\chi^z|\phi_\pm >= \pm\frac{1}{2}|\phi_\pm >$. Similarly the chiral-spin raising operator, along with its hermitian conjugate, is defined through $\chi^+|+>= 0, \chi^+|->= |+>$. We give the explicit form of the chirality operator $\vec{\chi}$ in terms of the spin operators below. This can be done with the help of the permutation operators.

Let the permutation operator P_1 denote the permutation $23 \rightarrow 32$. Similarly the operators P_2, P_3, permute 3 and 1, and 1 and 2 respectively. These permutation operators acting on one of the chiral states give the other chiral state modulo a phase. This implies that we should be able to construct the χ^+ and χ^- in terms of the P operators. The P operators are constructed easily from the original spin operators, for instance $P_1 = 2(\vec{s}_2.\vec{s}_3 + 1/4)$ and so on. The action of P_1 on the two chiral states can be seen easily, $P_1|+>= |->$ and $P_1|->= |+>$. This implies $P_1 = \chi^+ + \chi^- = 2\chi^x$. Similarly we can construct the other two operators, $P_2 = \kappa^2\chi^+\kappa\chi^-$ and $P_3 = \kappa\chi^+ + \kappa^2\chi^-$, where $\kappa = \exp(ik)$. It should be noted that the P operators are linearly dependent $P_1 + P_2 + P_3 = 0$, and they satisfy interesting commutator relations

$$\chi^z = \frac{1}{4i\sin k}[P_i, P_{i+1}] \tag{1}$$

for all i, and the anticommutator is -1. In fact this can be used as the definition of the chirality operator $\vec{\chi}$, in conjunction with $\chi^x = P_1/2$, and $i\chi^y = [\chi^z, \chi^x]$. Writing back the permutation operators in terms of the spin operators, we recover the box product form for χ^z. The advantage of writing $\vec{\chi}$ in terms of the permutation operators is that Eq.1 holds for any general N. The only difference is now $k = 2\pi/N$, and the permutation operators should be suitably constructed, which we illustrate below.

Before we come to the generalization of Eq.1, we present a simple understanding of the two-fold chiral degeneracy of Heisenberg chains using the Jordan-Wigner fermion representation of the spin operators[2]. Let $s_i^+ = c_i^\dagger \exp i\pi\sum_{j<i} n_j$, and $s_i^z = n_i - 1/2$, where c_i is a fermion annihilation operator at site i and n_i the fermion number operator. Under

this transformation the xy-part of the Heisenberg transforms into a fermion hopping term and the z-part becomes a nearest-neighbour interaction for the fermions. Let us focus on the xy-terms alone, as it turns out that the z-part of the Hamiltonian does not change the chiral degeneracy. The xy-part of the Heisenberg Hamiltonian reduces to $H_{xy} = J/2\sum_{i=1}^{N-1}(c_i^\dagger c_{i+1} + h.c.) + (-1)^{N_F+1}(c_1^\dagger c_N + h.c.)$. The periodic boundary condition of the closed chain gives rise to phase factor for the hopping amplitude between the sites 1 and N, which depends on the number of fermions $N_F = S^z + \frac{N}{2}$. The eigenstates of the above Hamiltonian are plain wave states, and the eigenvalues come in doublets except the lowest (or the highest depending on whether N_F is odd or even) eigenvalue. If we fill N_F states from below for $S^z = 1/2$ sector, for $S^z = -1/2$ the states get filled from above, and vice versa. In both cases the highest occupied doublets wil have only one fermion, which gives a degeneracy of two. Also there is a fermion current, and as the two eigenfunctions are related by a phase, the current changes direction between the two states. If we include the z-part of the Heisenberg Hamiltonian, the single-particle picture we have now does not hold. However, the single-particle current will translates into the motion of the center of mass, which means in the spin language that the center of mass of down (or up depending on the spin sector) spins moves around the chain in two directions, with a phase of $\exp \pm ikx_{cm}$, where x_{cm} is the coordinate of the center of mass. This can be seen explicitly for $N = 5$, from the Bethe anstaz states[3], though for general N it is quite involved.

With the above insight that the two chiral states differ by the phase of the motion of the center of mass of the down spins, we can now construct the permutation operators appearing in Eq.1. For a given site i we have an operator P_i which permutes the spin labels such that $i + j \to N + i - j$. This is equivalent to doing a reflection on a regular polygon with N sites, around a straightline bisecting the angle at site i. For instance in the case of $N = 5$, the operator P_1 permutes the spin labels $12345 \to 15432$, and P_2 does the permutation $12345 \to 32154$ and so on. The P operators can be readily constructed from the spin operators, as each of them involve $(N-1)/2$ pair-wise permutations, as

$$P_i = 2^{\frac{N-1}{2}} \prod_{j=1}^{\frac{N-1}{2}} (s_{i+j}.s_{N+i-j} + \frac{1}{4}). \tag{2}$$

We need to relate these permutation operators to the chiral-spin raising and lowering operators, which will give us the desired construction of the chiral operator $\vec{\chi}$ in terms of the spin operators. Let us label the spins on a closed chain such that $P_1|\pm>=|\mp>$, implying $P_1 = \chi^+ + \chi^-$, as we have seen in the case of three spins. The action of the other P operator can be seen from the action of the cyclic permutation operator R, which permutes the spin labels such that $i \to i+1$. The R operator shifts all the spin labels by one unit, which gives a shift of one unit for the center of mass of the down spins, *i.e.* $R|\pm>=\exp(\mp ik)|\pm>$. Let $|\tilde{+}>=\kappa^*|+>, |\tilde{-}>=\kappa|->$, where $\kappa = \exp ik$. The action of P_2 on these new states $|\tilde{\pm}>$ is similar to the action of P_1 on $|\pm>$, *i.e.*$P_2|\tilde{\pm}>=|\tilde{\mp}>$. This gives us $P_2 = \kappa^*\chi^+ + \kappa\chi^-$. Now using the operator R again, we can construct P_3, and the procedure can be repeated to get the other operators. In a concise notation we have P_i given as

$$P_i = A_i^*\chi^+ + A_i\chi^-,$$

where $A_i = \kappa^i$. The commutator relation between P_i, P_{i+1} remain the same the same as in the case of three spins as given in Eq.1. More generally we have

$$[P_l, P_{l+m}] = 4i\chi^z \sin mk, \tag{3}$$

and the anticommutator is $2\cos mk$. This completes the construction of the chirality operators, Eq.2 and Eq.3, in terms of the spin operators. It is interesting to note that for each of the permutation operator $[P_i, H] = 0$, this is because the Hamiltonian is invariant under an anticyclic permutation. This implies the chirality operators, as they involve only the permutation operators explicitly, commute with the Hamiltonian.

Now we would like to comment on the closed chain with an even number of sites. For even N the ground state of Heisenberg antiferromagnet belongs to $S=0$ sectors, and is nondegenerate. It is also easy to see from the Jordon-Wigner transformation we discussed above. For $N = 2n$, the number of fermions is $N_F = n$. For n even the eigenvalues spectrum for the $xy-$part consists of n doublets, and the ground states is nondegenerate with $n/2$ doublets filled in. For odd n the eigenvalue spectrum consists of nondegenerate highest and lowest energy states and the rest of the states in doublets, and the ground state is again nondegenerate with $(n-1)/2$ doublets and the lowest nondegenerate state filled in. This implies $\chi^z = 0$. However this situation is not analogous to the $S = 3/2$ excited states of a triangle with $\chi^z = 0$. The difference is that for the case of three spins (or for any odd N) the chirality operator exists, and still there could be states with $\chi^z = 0$, while for for even N the chirality operator does not exist, *i.e.* $\chi^z \equiv 0$. For example consider $N = 4$, which is the simplest nontrivial case. It is easy to see that $P_1 = P_3$, as in both cases only one pair of spin labels 2 and 4 have to be permuted. We have $[P_1, P_2] = [P_2, P_3]$, implying $\chi^z \equiv 0$. This argument can be readily generalized for any even N. Noting that $P_i = P_{\frac{N}{2}+i}$, from the commutator relations of Eq.3 for $\{l = 1, m = \frac{N}{2} - 1\}$ and $\{l = \frac{N}{2}, m = 1\}$, we have $\chi^z = -\chi^z$, which implies the chirality does not exist.

In summary, we have constructed the chirality operators for the two-fold chiral ground states of Hiesenberg antiferromagnetic chains with odd number of sites explicitly in terms of the spin operators. It would be interesting to see if chirality operators can be constructed independent of the interaction between the spin degrees of freedom.

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