New Types of Off-Diagonal Long Range Order in Spin-Chains

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(October 20, 2018)

Abstract

We discuss new possibilities for Off-Diagonal Long Range Order (ODLRO) in spin chains involving operators which add or delete sites from the chain. For the Heisenberg and Inverse Square Exchange models we give strong numerical evidence for the hidden ODLRO conjectured by Anderson [1]. We find a similar ODLRO for the XY model (or equivalently for free fermions in one spatial dimension) which we can demonstrate rigorously, as well as numerically. A connection to the singlet pair correlations in one dimensional models of interacting electrons is made and briefly discussed.
In 1991 one of us (P.W.A) conjectured, based on RVB ideas for the one-dimensional Hubbard model, that there should be a non-zero overlap between the groundstate of the one dimensional Heisenberg model on a chain of \( N \) sites and the state obtained by inserting a pair of nearest neighbor spins in a singlet configuration into the ground state of the \( N-2 \) site Heisenberg chains [1,2]. Both of these models were therefore expected to have a hidden form of ODLRO for an operator which not only involved sampling the state of the system (in this case checking that a given pair of spins was in a singlet) but also changing the Hilbert space of the system in an essential way (adding two sites), reminiscent of the Girvin-MacDonald-Read order parameter of the Fractional Quantum Hall Effect (FQHE) [3], despite the fact that the Heisenberg model has gapless excitations. The conjecture that the overlap should be finite has not been previously investigated (but see [4] where evidence for the resulting ODLRO was found); therefore we numerically tested the original conjecture that the overlap for the ISE and Heisenberg models between the \( N \) site groundstate and the \( N-2 \) site groundstate with a local singlet inserted should be non-zero.

These overlaps as a function of \( N \) are shown in Fig. 1 together with fits to the results of the form \( 0.817 + 0.778N^{-2} \) for the ISE model and \( 0.820 + .740N^{-2} \) for the Heisenberg model. The results strongly suggest that both overlaps remains finite in the limit as the system size goes to infinity. Note that since the phases of the \( N \) and \( N-2 \) site wavefunctions may be chosen independently the phase of the overlaps is meaningless and further, since the groundstate momenta of the \( N \) and \( N-2 \) site groundstate wavefunctions differ by \( \pi \), the overlap is multiplied by minus one if the location of the singlet pair is shifted by one site. We have chosen the overlap real and positive for convenience.

As Fig. 1 shows, the overlaps in the ISE and Heisenberg models are not only finite in the \( N \to \infty \) limit, but also surprisingly close to each other, despite the fact that the ranges of the interaction in both models are quite different. We now present an analytical calculation in the ISE model that gives some understanding of origin of this finite number. The groundstate wavefunction of the ISE model in a basis of local spins \( \{|\sigma_1 \cdots \sigma_M\}\), \( \sigma_i = \pm \frac{1}{2} \) is given by [5]:
\[ \Psi_M^n{\sigma_1 \cdots \sigma_M} = \prod_{i<j}^{M}(z_i - z_j)^{\delta_{\sigma_i \sigma_j}} e^{\frac{i}{2} \text{sgn}(\sigma_i - \sigma_j)}. \]  

For the \(N\) site ISE groundstate \(M = N\) and \(\{z_i\} \equiv C_N = \{e^{\frac{2\pi i n}{N}}\}_{n=1}^N\), while for the \(N - 2\) site groundstate \(M = N - 2\) and \(\{z_i\} \equiv C_{N-2} = \{e^{\frac{2\pi i n}{N-2}}\}_{n=1}^{N-2}\). To compute the ISE overlap we add \(\sigma_{N-1}, \sigma_N\), sitting in a singlet, to the \(N - 2\) site groundstate. This overlap is hard to calculate since the \(z_i\)'s from both sets are not commensurate with each other. However, if we slightly deform the set \(C_{N-2}\) to be \(\{e^{\frac{2\pi i n}{N-2}}\}_{n=1}^{N-2}\) and leave \(\sigma_{N-1}, \sigma_N\) in a singlet then we obtain a new state \(\Psi^2_N\), that can be recognized as a localized 2-spinon state [6, 7]. Spinons are the elementary excitations of the ISE model with semionic statistics [6]. Although this localized spinon state is not an energy eigenstate it consists of an admixture of eigenstates that contain only 0 spinons (the groundstate on \(N\) sites) or 2 spinons. Here the localized spinons sit at sites \(N - 1\) and \(N\) in a singlet. In general we could have put them at sites \(\alpha, \beta\) by deforming \(C_{N-2}\) into \(\{e^{\frac{2\pi i n}{N}}\}_{i=1}^{N}/\{e^{\frac{2\pi i n}{N}}, e^{-\frac{2\pi i n}{N}}\}\). 

In the basis of states with \(M\) overturned spins with respect to the ferromagnetic state labeled by their positions along the chain: \(n_1, \ldots, n_M\), \(\Psi^0_N\) and \(\Psi^2_N\) are given by:

\[ \Psi^0_N(n_1, \ldots, n_M) = \prod_{i=1}^{N/2} (-)^{n_i} \prod_{i<j}^{N} \sin^2 \left( \frac{n_i - n_j}{N} \pi \right) \]  

\[ \Psi^2_N(n_1, \ldots, n_M - 1) = \prod_{i=1}^{N/2 - 1} (-)^{n_i} \prod_{i<j}^{N} \sin^2 \left( \frac{n_i - n_j}{N} \pi \right) \times \prod_{i=1}^{N/2 - 1} \sin \left( \frac{n_i - \alpha}{N} \pi \right) \sin \left( \frac{n_i - \beta}{N} \pi \right) \]  

We now calculate the overlap between \(\Psi^0_N\) and \(\Psi^2_N\) for arbitrary separation \(\alpha\) between the spinons (because of translational invariance we can fix \(\beta\) to be 0). We have for the overlap:

\[ \frac{\langle \Psi^0 | \Psi^2(\alpha) \rangle}{\sqrt{\langle \Psi^0 | \Psi^0 \rangle \langle \Psi^2(\alpha) | \Psi^2(\alpha) \rangle}} = \frac{\langle \Psi^0 | \Psi^2(\alpha) \rangle}{\langle \Psi^0 | \Psi^0 \rangle} \left( \frac{\langle \Psi^2(\alpha) | \Psi^2(\alpha) \rangle}{\langle \Psi^0 | \Psi^0 \rangle} \right)^{-\frac{1}{2}} \]  

First we will determine \(\langle \Psi^0 | \Psi^2(\alpha) \rangle\). Setting \(M = \frac{N}{2} - 1\):

\[ \langle \Psi^0 | \Psi^2(\alpha) \rangle = \left(\frac{N}{2}\right)! \sum_{n_1, \ldots, n_M} \Psi^2(n_1, \ldots, n_M | 0, \alpha) \times \]
\[
\left\{ \Psi^0(n_1, \ldots, n_M, 0) - \Psi^0(n_1, \ldots, n_M, \alpha) \right\}^* = \left( \frac{N}{2} \right)! \sigma(\alpha) (1 - (-)^\alpha).
\]

Here
\[
\sigma(\alpha) = \sum_{n_1, \ldots, n_M} \left( \prod_{i<j} \sin^4 \left( \frac{n_i - n_j}{N} \right) \right) \times \prod_{i=1}^M \sin^3 \left( \frac{\pi n_i}{N} \right) \prod_{i=1}^M \sin \left( \frac{n_i - \alpha}{N} \right).
\]

In eq. (5) we shifted all the \( n_i \) by \( \alpha \) in the second term to bring both terms in the same form.

Since \( \Psi^0 \) is a singlet we know that if the two spinons in \( \Psi^2 \) were in the \( S_z = 0 \) triplet state the overlap should be zero, i.e. \( \langle \Psi^0 | \Psi^2(\alpha) \text{, triplet} \rangle \propto \sigma(\alpha) (1 + (-)^\alpha) = 0 \) for all \( \alpha \). Therefore \( \sigma(\alpha) \) vanishes for all even \( \alpha \). At the same time we see from eq. (6) that \( \sigma(\alpha) \) is a polynomial in \( \cos \left( \frac{\pi \alpha}{N} \right) \). This is easily checked by expanding the \( \sin \left( \frac{n_i - \alpha}{N} \right) \) and noting that \( \sigma(\alpha) \) is even in \( \alpha \). We conclude immediately:
\[
\sigma(\alpha) \propto \prod_{j=1}^{N/2} \left( \cos \left( \frac{\pi \alpha}{N} \right) - \cos \left( \frac{2\pi j}{N} \right) \right) \propto \frac{\sin \left( \frac{\pi \alpha}{2} \right)}{\sin \left( \frac{\pi \alpha}{N} \right)}.
\]

Now we turn our attention to the second piece. Only its numerator is \( \alpha \) dependent:
\[
\langle \Psi^2(\alpha) | \Psi^2(\alpha) \rangle = 2 \left( \frac{N}{2} - 1 \right)! \sum_{\{n_1, \ldots, n_M\}} \left( \Psi^2(n_1, \ldots, n_M | 0, \alpha) \right)^2 = 2 \left( \frac{N}{2} - 1 \right)! \sum_{n_1, \ldots, n_M} \prod_{i<j} \sin^4 \left( \frac{n_i - n_j}{N} \right) \times \prod_{i=1}^M \sin^2 \left( \frac{\pi n_i}{N} \right) \sin^2 \left( \frac{n_i - \alpha}{N} \right).
\]

But this sum can be recognized as the \( \langle S_z(\alpha)S_z(0) \rangle \) static correlation function in the ISE model [2], or—after an (exact) conversion of the sums to integrals—as the one-particle density matrix in the Calogero-Sutherland model at half filling [8]. The result for large \( N \) is
that is proportional to $\frac{\text{Si}(\pi \alpha)}{\pi \alpha}$, where $\text{Si}(x)$ is the sine-integral function. The entire expression for the overlap, with normalization computed by considering $\alpha = 0$, then becomes:

$$
\frac{2 \sin \left( \frac{\pi \alpha}{2} \right)}{N} \sqrt{\frac{\pi \alpha}{\text{Si}(\pi \alpha)}},
$$

(9)

Thus for a nearest neighbor the overlap is $2 \pi \sqrt{\frac{\pi}{\text{Si}(\pi)}} \approx 0.82917$, which is within 1.5% of the Heisenberg and ISE groundstate singlet insertion overlaps.

Many of the properties of the two spinon matrix element can be understood in terms of the Girvin-MacDonald-Read [3] order parameter for the bosonic $\nu = \frac{1}{2}$ Laughlin [9] state. In the spinon language, the insertion of up-spin spinons acts on the down-spin wavefunction in that same way as the quasi-hole operator of the $\nu = \frac{1}{2}$ state, while the insertion of a down-spin spinon acts analogously to the insertion of a quasi-hole and a hard-core boson.

Consequently, the two spinon insertion for $\alpha = 0$ clearly takes the bosonic $\nu = \frac{1}{2}$ state with $\frac{N}{2} - 1$ particles, periodic on a ring of size $N - 2$, to the $\nu = \frac{1}{2}$ state with $\frac{N}{2}$ particles periodic on a ring of size $N$, and is essentially the Girvin-MacDonald-Read order parameter for the $\nu = \frac{1}{2}$ state and the overlap associated with it must be identically equal to one.

Further, for $\alpha \neq 0$, the two spinon insertion is equivalent to a sum of two operators: a quasi-hole being inserted a finite distance from a hard core boson and another quasi-hole. Such an object should still have an expectation value given essentially by the quasihole propagator. This would decay exponentially in the bulk of a $\nu = \frac{1}{2}$ state, but near the edge would decay only as $\alpha^{-\frac{1}{2}}$, exactly as the two spinon matrix element does (see Eq. (1) and Fig. 2). The vanishing of the matrix element for any even $\alpha$ and its alternation for odd $\alpha$ simply reflect the lattice structure of our model, the phase of the quasi-hole propagator and the fact that the spinon operator is a superposition of two operators so that the result is real, rather than complex. The reason why the two spinon overlap agrees so well with the actual singlet insertion overlap is unclear, however, our numerical Monte Carlo results for the singlet insertion display the same power law decay as a function of the spin separation (see figure 2). The insertion overlap also vanishes for separations which are even multiples of the lattice spacing and alternation for separations which are odd multiples of the lattice spacing.
spacing, so it would appear that for the Heisenberg and ISE models the spin chain ODLRO is essentially that same as the ODLRO of the $\nu = \frac{1}{2}$ Laughlin state.

Note that, since the two spinon insertion operator generates states with either zero or two spinons, the zero spinon state being the ground state, its action is analogous to the action of a pair of fermionic creation and annihilation operators on the fermionic groundstate, generating states which contain one particle and one hole or else no particles and holes, i.e. the groundstate. The matrix element to the ground state as a function of the space-time separation of the fermionic creation and annihilation operators is the amplitude for the fermion to propagate to the space-time location where it can be annihilated and is by definition the fermion propagator. The overlap we calculate is, by analogy, proportional to the equal time spinon propagator, i.e. the amplitude for either of the spinons to propagate to the location of the other, at which point the two can annihilate each other, provided they are in a singlet configuration.

In an effort to better understand our results for the Heisenberg and ISE models, we examined the overlap for the same insertion operator acting on the $N - 2$ site $XY$ model groundstate with the $N$ site $XY$ model groundstate. The strikingly similar result, here extended to a larger system size than was possible for the Heisenberg and ISE models, is shown in Fig. 1. Since the $XY$ model can be mapped onto spinless fermions, the “order parameter” can be recast in that language and a more detailed study made. In that language the non-zero overlap is between the groundstate for $N/2$ spinless fermions, with either periodic or antiperiodic boundary conditions, on $N$ sites (with positive hopping integral so that their momenta in the groundstate are centered around $\pi$) and the state obtained by adding two sites and one fermion (in a superposition of being on the two added sites with a relative minus sign for the two different sites) to the groundstate for the $N/2 - 1$ spinless fermions on $N - 2$ sites—with the opposite boundary conditions from the $N$ site case. The change of boundary conditions is a non-local operation in the fermion language, however in the spin language it arises from a local operation, i.e. the insertion of two additional spins in a singlet configuration.
Since the wavefunctions for the two fermion states to be overlapped are those of free particles, considerable progress can be made in its computation. In particular, it can be bounded rigorously from below. The calculation is straightforward, using simple properties of polynomials which roots lie on the unit circle, and the fact that the corresponding momenta for the $N-2$ and $N$ site models differ only by $O(1/N^2)$ near the Fermi surface. We will present the proof elsewhere. Here we state only the result that the lower bound obtained was $e^{-\frac{5}{2}} + O(N^{-1})$.

The non-zero overlap for the XY model is particularly striking since we know that the overlap between the $N$ site, $\frac{N}{2}$ particle groundstate and the state created by inserting a single, localized electron into the $N$ site, $\frac{N}{2}-1$ particle groundstate would vanish like $N^{-\frac{1}{2}}$, while the overlap between the $N$ site, $\frac{N}{2}$ particle groundstates between models with periodic and antiperiodic boundary conditions vanishes like $N^{-1}$.

The vanishing of the overlap for the insertion of a single, localized fermion implies that no analog of the two spinon calculation exists for the XY model, since the only way to make the momenta similar in the two overlapped states is to make $\frac{N}{2}-1$ of them identical is which case the overlap will vanish like $N^{-\frac{1}{2}}$.

It may appear that, since the “order parameter” we have defined involves spin chains with different numbers of sites, there will be no physical consequences to this form of ODLRO and in fact there is, for example, no additional groundstate degeneracy associated with the existence of this kind of order. However, order of the type we find can have important consequences for more general models than spin chains. For example, we will now show that the ODLRO of the Heisenberg model is responsible for the leading contribution to the singlet pair susceptibility of the one dimensional Hubbard model and is thus not without potentially important physical consequences.

First, we make the connection between the ODLRO found for the Heisenberg model and the equal time, singlet pairing correlation function of the one dimensional Hubbard model in the limit as $U \to \infty$. In that limit the groundstate wavefunction of the Hubbard model is given by a product of spin and charge wavefunctions, the latter being given by a spinless
fermion determinant and the former by a Bethe Ansatz wavefunction for the “squeezed” Heisenberg model, i.e. a Heisenberg model defined only on those sites occupied by the spinless fermions \[11\]. For periodic boundary conditions and the number of electrons equal to \(4N + 2\), \(N\) an integer, the ground state wavefunction for the Heisenberg model should be used. The equal time singlet pair correlation function is given by the overlap of the groundstate with the state obtained from the groundstate by removing a nearest-neighbor, singlet pair of electrons at sites which we can take to be 0 and 1 and then inserting a nearest-neighbor, singlet pair of electrons at sites \(j\) and \(j + 1\). Due to the hidden ODLRO of the Heisenberg model, the spin wavefunction overlap for a fixed charge-configuration has a piece which for large separation, \(j\), is just given by a constant times \((-1)^{n_j}\), where \(n_j\) is the number of spinless fermions found on sites between 1 and \(j\) in that charge configuration. This leads to a contribution to the correlation function which is given by the expectation value in the spinless fermion groundstate of \(\Psi(j + 1)\Psi(j)\Psi(1)\Psi(0)(-1)\sum_{j > l > 1} \Psi^\dagger(l)\Psi(l)\), similar to the correlation function for the alternating, spin-spin correlation function studied by Sorella, et al. \[12\]. The leading asymptotic behavior of this expectation value can be computed straightforwardly from Abelian bosonization and is given by \(A \cos(k_F x) x^{-5/2}\), where \(k_F\) is the \(k_F\) of the spinless fermions and \(A\) is a cutoff dependent constant. This agrees with the predictions of the Luttinger liquid description of the Hubbard model \[13,17\], provided that we take the charge sector rediagonalization parameter, \(K_\rho\), to be 1/2 and remember that the \(k_F\) of the spinless fermions is twice that of electrons with spin at the same filling fraction.

In the Hubbard model, this contribution to the singlet pair correlation functions arises because the bosonized form of \(\psi_\uparrow(j)\psi_\downarrow(j + 1)\) contains an operator proportional to \(\exp(i\Theta_{R,\rho})\), involving only charge degrees of freedom. \[13\]. This operator is present because the operator product expansion for \(\exp\left(\frac{i}{2}\Theta_{R,\sigma}(x)\right)\exp\left(-\frac{i}{2}\Theta_{R,\sigma}(x')\right)\) contains the identity times a coefficient asymptotically proportional to \((x - x')^{-1/2}\). The decay of this coefficient with separation implies that, if the electrons are inserted \(m\) sites apart where \(m \gg 1\) but \(j \gg m\), the singlet pair correlations decay with \(j\) in the same way, but there is a multiplication of the prefactor, \(A\), by a factor of \(m^{-1/2}\) arising from spin degrees of freedom \[14\]. This is in in agreement with
the decay we find for the singlet and two spinon insertions in the ISE and Heisenberg models, and suggests the identification of the insertion of an up-spin spinon into the ISE model with the action of the operator 

\[ O_{\text{insert}} = i^j \exp \left( \frac{i}{2} \Theta_{R,\sigma}(j, a) \right) + (-i)^j \exp \left( \frac{i}{2} \Theta_{L,\sigma}(j, a) \right), \]

where \( a \) is the lattice spacing and \( j \) is the number of sites to the left of the insertion site in the original chain. Since this operator is a semion, it is natural to identify it as the spinon creation operator; an identification compatible with the observation of [15] that the generalized commutation relations of the Fourier modes of this operator provide a natural realization of the Yangian.

The identification is also compatible with the alternation with odd separation and vanishing for even separation that we find for the singlet and two spinon insertions. Both are in agreement with the singlet pair correlations of the Hubbard model as computed with Abelian bosonization.

The connection to Abelian bosonization should be extendable to generalizations of the Hubbard model which include spin-dependent interactions so that the Luttinger liquid rediagonalization parameter of the spin sector of the Hubbard model, \( \kappa_{\sigma} \) (for a definition of \( \kappa_{\sigma} \) see [16]) is renormalized from 1. At half filling the low energy sector of the model then becomes a general XXZ model. This would change the exponent for the decay of the singlet insertion overlap from \( \frac{1}{2} \) to an exponent, \( \eta = \frac{1}{4}(\kappa_{\sigma} + \kappa_{\sigma}^{-1}) \). For XXZ models this is a simple function of the anisotropy of the model [18]. In general: \( \kappa_{\sigma} = 1 - \frac{1}{2} \cos^{-1} \left( \frac{J_{xy}}{J_{zz}} \right) \). This is equal to \( \frac{5}{8} \) at the XY point exactly as we observe. Based on the connection between the two spinon overlap and the singlet insertion for the ISE model, where spinons are noninteracting, we argued that the decay exponent was just the exponent of the spinon-spinon propagator.

We note that that the alternating piece in the singlet-pair correlation function is the slowest decaying piece of that correlation function for the Hubbard model and may have important consequences for superconducting correlations in models based on the one dimensional Hubbard model. In particular, if one considers an array of Hubbard chains coupled...
with operators which properly correlate the positions of the electrons on neighboring chains without disrupting the singlet overlap property or the charge degrees of freedom greatly then the scaling dimension of pair hopping between the chains will be renormalized and pair hopping will become relevant and lead to an instability similar to that envisioned in the interlayer tunneling mechanism for superconductivity. Relevant operators having this effect occur naturally when the spin-spin superexchange interaction between chains is considered in the bosonization language [19].

We gratefully acknowledge helpful correspondences with M. Ogata and discussions with F. D. M. Haldane and D. G. Clarke, as well as financial support from NSF grants DMR-9104873 (P. W. A.) and DMR-922407 (J. C. T.) and the NEC corporation (S. P. S.).
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[14] This is more than offset by a charge degree of freedom induced renormalization of $A$ by $m^\pm\frac{2}{5}$, which can be derived from either the Ogata-Shiba wavefunction or the Luttinger liquid description of the large $U$ Hubbard model.

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FIGURES

FIG. 1. Calculated Overlap for the ISE and Heisenberg Models

Shown are the calculated overlaps between the $N$ spin groundstate of the $1/r^2$, nearest neighbor Heisenberg and $XY$ models and the states obtained by inserting a nearest neighbor singlet pair of spins into the $N - 2$ spin groundstates of those models. The dashed line is a fit to the ISE results using $0.0817 + 0.778N^{-2}$, the solid to Heisenberg results using $0.820 + 0.740N^{-2}$, and the dotted and dashed a fit to the $XY$ results using $0.808 + .819N^{-2}$.

FIG. 2. The Decay with Separation of the Overlap

The exact overlap for the $XY$ and the Monte Carlo calculated overlap for the ISE model as functions of the system size for spins inserted in a singlet configuration separated by half the size of the system. The results obtained in this way should be purely power law in the large system size limit, whereas correlation functions at fixed system size generally deviate from power law when the separation is not small compared to the system size. We have also examined correlation functions at fixed system size, and exact results for smaller systems for the ISE and Heisenberg models. All of those produced results consistent with $\alpha^{-\frac{1}{2}}$ behavior for the ISE and Heisenberg models and $\alpha^{-\frac{5}{8}}$ behavior for the $XY$ model.
Overlap (singlet size = 1)

- Heisenberg data
- Heisenberg fit
- ISE data
- ISE fit
- XY data
- XY fit
Overlap (singlet size = N/2)

ISE scaling-data
ISE scaling-fit
XY scaling-data
XY scaling-fit

slope = 0.50
slope = 0.625