A chiral spin liquid wave function and the Lieb-Schulz-Mattis theorem

Sandro Sorella, Luca Capriotti, Federico Becca, and Alberto Parola

1 INFN-Democritos, National Simulation Center, and SISSA, I-34014 Trieste, Italy
2 Kauffman Institute for Theoretical Physics, University of California, Santa Barbara CA 93106-4030
3 Istituto Nazionale per la Fisica della Materia and Dipartimento di Scienze, Università dell’Insubria, I-22100 Como, Italy

(Dated: January 9, 2022)

We study a chiral spin liquid wave function defined as a Gutzwiller projected BCS state with a complex pairing function. After projection, spontaneous dimerization is found for any odd but finite number of chains, thus satisfying the Lieb-Schultz-Mattis theorem, whereas for even number of chains there is no dimerization. The two-dimensional thermodynamic limit is consistently reached for large number of chains since the dimer order parameter vanishes in this limit. This property clearly supports the possibility of a spin liquid ground state in two dimensions with a gap to all physical excitations and with no broken translation symmetry.

PACS numbers: 74.20.Mn, 71.10.Fd, 71.10.Pm, 71.27.+a

A long time after its first proposal, the existence of a spin liquid ground state (GS) in two-dimensional (2D) quantum spin one-half models is still a very controversial issue. This is mainly because all one-dimensional (1D) or quasi-1D spin models that can be solved exactly, either numerically or analytically, display a gap to the spin excitations only when a broken translation symmetry is found in GS (e.g., in spin-Peierls systems) or when the unit cell contains an even number of spin 1/2 electrons (e.g., in the two-chain Heisenberg model). Hence, in these models the electronic correlations do not play a crucial role since their GS can be adiabatically connected to a band insulator without any transition. This important property of insulators, which clearly holds in 1D systems, has been speculated to be generally valid even in higher dimensions, as it appears to follow from a general result, the Lieb-Schultz-Mattis (LSM) theorem, whose range of validity has been extended to more interesting 2D cases.

Recently, there has been an intense theoretical and numerical investigation of non-magnetic wave functions obtained after Gutzwiller projection of the GS of a BCS Hamiltonian. On a rectangular \(L_x \times L_y\) lattice, this state can be written in the following general form:

\[
|p-BCS\rangle = \hat{P}_G \left[ \sum_k f_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger \right]^N |0\rangle ,
\]

where \(N\) is the number of electrons (equal to the number of sites, i.e., \(N = L_x \times L_y\)), \(\hat{P}_G\) is the Gutzwiller projection onto the subspace of no doubly occupied sites, and \(c_{k,\uparrow}^\dagger\) and \(c_{k,\downarrow}^\dagger\) are creation operators of a spin up or a spin down electron, respectively. These are defined in a plane-wave state with momentum \(k\) allowed by the chosen boundary conditions: periodic (PBC) or antiperiodic (APBC) in each direction. It is worth noting that, after the projection, the wave function corresponds to PBC on the spin Hamiltonian, regardless the choice of boundary conditions on the electronic states. The pairing function \(f_k\) can be easily related to the gap function \(\Delta_k\) and the bare dispersion \(\epsilon_k = -2(\cos k_x + \cos k_y)\) of the BCS Hamiltonian:

\[
\hat{H}_\text{BCS} = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_k (\Delta_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger + \text{h.c.}) ,
\]

by means of the simple relation \(f_k = \Delta_k/|\epsilon_k + E_k|\), where the gap function \(\Delta_k\) can be in general any complex function even under inversion \(\Delta_k = \Delta_{-k}\), as required here for a singlet wave function. \(E_k\) and \(E_k = \sqrt{|\Delta_k|^2 + \epsilon_k^2}\) represents the spin-half excitation energies of \(\hat{H}_\text{BCS}\).

As clearly pointed out by Wen, in presence of a finite gap \(\Delta_{BCS}\) in the thermodynamic limit, such that \(E_k \geq \Delta_{BCS} > 0\), the corresponding BCS finite correlation length is expected to be robust under Gutzwiller projection. Here, we restrict to this class of non-magnetic states, considering the projected BCS (\(p\)-BCS) state which is obtained by a \(d + id\) gap function of the following form:

\[
\Delta_k = \Delta x_x y_y (\cos k_x - \cos k_y) + i \Delta_{xy} \sin k_x \sin k_y .
\]

This wave function breaks the time reversal symmetry \(\hat{T}\) and the parity symmetry \((x \leftrightarrow y)\) \(\hat{P}\), whereas \(\hat{T} \otimes \hat{P}\) is instead a well defined symmetry. Hence, this spin liquid wave function may have a non-vanishing value of the so-called \(\text{chiral}\) order parameter:

\[
\hat{O}_C = \frac{1}{N} \sum_{i} \hat{S}_i \cdot (\hat{S}_{i+d_x} \times \hat{S}_{i+d_y}) ,
\]

with \(d_x = (1,0)\) and \(d_y = (0,1)\). Chiral spin liquids were introduced a long time ago, however, to our knowledge, this is the first attempt to represent this class of states in the \(p\)-BCS framework. On finite size systems, we take the real part of the complex wave function, so that all the finite-size symmetries, including parity, are satisfied and a spontaneously broken lattice symmetry can occur only in the thermodynamic limit.
In the following we consider in more detail the relation of the p-BCS wave functions with the LSM theorem. Given a short-range spin Hamiltonian $H$, on a $L_x \times L_y$ rectangle (PBC on the $x$ direction are assumed) and a variational state $|\psi_0\rangle$ with given momentum, we can define another variational state, $|\psi'_0\rangle = \hat{O}_{LSM} |\psi_0\rangle$, by means of the LSM operator:

$$\hat{O}_{LSM} = \exp \left[ i \sum_r 2 \pi x/L_x \hat{S}_r^z \right] ,$$

where $r = (x, y)$ indicates the position of each site on the lattice. The new variational state $|\psi'_0\rangle$ has the following properties:

1. Its energy expectation value differs at most by $O(L_y/L_x)$ from the variational energy of $|\psi_0\rangle$.
2. If $L_y$ is odd, regardless of the boundary conditions on the $y$ direction, the momenta parallel to $x$ corresponding to $|\psi_0\rangle$ and $|\psi'_0\rangle$ differ by $\pi$. Hence: $\langle \psi'_0 | \psi_0 \rangle = 0$.

For 1D or quasi-1D system with odd number of chains $L_y$ and vanishing aspect ratio ($L_y/L_x \to 0$ for $L_x \to \infty$), by applying the LSM operator to the actual GS, it is possible to construct an excitation of the system with momentum $(\pi, 0)$ which becomes degenerate with the GS in the thermodynamic limit. This implies in turn either a gapless spectrum or, in presence of a finite gap, a twofold degenerate GS with a doubling of the unit cell and a spontaneously broken translation symmetry. For instance, the presence of a singlet zero-energy excitation with momentum $(\pi, 0)$ is just a characteristic of spontaneous spin-Peierls dimerization, as it appears for example in the Majumdar-Gosh chain. This result, holding rigorously in the limit of vanishing aspect ratio, has been argued to apply in general for 2D systems. In the following, we will show, with an explicit example, that this result in 2D does not necessarily imply spontaneous dimerization, but topological degeneracy of the GS.

It is simple to show that $O_{LSM} |p-BCS\rangle = |p-BCS'\rangle$, namely the same type of wave function of Eq. 11 is obtained, with the changes below:

$$k \to \tilde{k} ,$$

$$f_k \to \tilde{f}_k = f_{k-(\pi/L_x,0)} = f_{\tilde{k}} ,$$

where the new quantized momenta $\tilde{k} = k + (\pi/L_x,0)$ are obtained by interchanging PBC with APBC in the $x$ direction only and Eq. 7 means that the pairing function is calculated with the old momenta $k$: $f_k c_{k,\uparrow}^\dagger c_{\tilde{k},\downarrow}^\dagger$. By definition, the wave function $|p-BCS'\rangle$ has therefore the same quantum numbers predicted by the LSM theorem, the change of momentum being implied by Eq. 6. The reason why the momentum of the wavefunction 11 can be non zero for odd number of chains is indeed rather subtle but easy to verify. Indeed the $x-$translation operator with APBC translates all creation operators, but the ones belonging to the boundary are also multiplied by a phase factor $(-1)$. This translation operator always leaves invariant the $|p-BCS\rangle$ wave function. However, for a spin state with one electron per site each configuration has always $L_y$ electrons at the boundary, so that the physical spin translation operation (defined with PBC), differs from the APBC one for an overall phase $(-1)^{L_y}$, namely a momentum $(\pi, 0)$ for odd number of chains. Analogously, the excitations obtained by modifying only the boundary conditions in the BCS Hamiltonian (in the $x$ and/or $y$ direction), namely using Eq. 6 (and/or its equivalent for the $y$ direction) and $f_k \to \tilde{f}_k$, may display in 2D the topological degeneracy of this spin liquid wave function.

We now assume that the the p-BCS wave function 11 with the $\Delta_k$ given by Eq. 3 represents the GS of some short-range Hamiltonian. However, here we do not address the question whether this chiral wave function can be stabilized in some physical Hamiltonian. Certainly explicit Hamiltonians with short-range off-diagonal matrix elements can be constructed by a simple inversion problem scheme. Having a finite gap $\Delta_{BCS}$, this wave function describes a spin system with a finite correlation length, and consequently a finite triplet gap. The LSM theorem can be then applied in the geometries where it holds, like, for instance, the three-leg ladder with PBC in both directions. As shown in Fig. 1, it is clear that spontaneous dimerization is obtained in the thermodynamic system for this geometry, as the dimer-dimer correlation functions on each chain, $\Delta(r - r') = \langle \hat{S}^z_r \hat{S}^z_{r+d_x} \hat{S}^z_{r+d_y} \hat{S}^z_{r+d_x+d_y} \rangle$, behaves for large distance as $(-1)^{r-x}O_{SP}/6\theta + \text{const.}$, being $O_{SP}$ the dimer order parameter. In strong
analogy with the one-dimensional Heisenberg chain in the gapped phase, the broken translation symmetry allows the system to satisfy the LSM theorem. In fact, it implies two degenerate singlet states with momentum differing by $(\pi, 0)$. In contrast, on any even-leg ladder, where the LSM theorem does not imply the degeneracy, the $p$-BCS state does not break translational invariance, as illustrated in Fig. 4 for the four-leg system. Despite the dichotomy between the odd and even chain cases, the 2D thermodynamic limit can be still consistently defined. In fact, as it is clearly shown in Fig. 4 though a finite dimer order parameter is obtained for any odd chain ladder, the order parameter is exponentially decreasing with the number of chains [see Fig. 4]. This implies that the broken symmetry, which is correctly obtained for odd but finite number of chains, represents an irrelevant effect in the 2D thermodynamic system. Nonetheless, in the 2D system, the GS can possess degenerate topological excitations. For instance, the matrix element of the dimer operator with momentum $(\pi, 0)$ between the two degenerate singlet states, which is finite on any finite number of chains, decreases exponentially with increasing $L_y$, as it is bounded by order parameter (see Fig. 4). Remarkably, the chiral order parameter remains instead a genuine feature of this variational wave function even in the 2D limit, as shown in Fig. 3 where an order parameter $O_C = \sqrt{\langle O_C^2 \rangle} \simeq 0.03$ was found for this wave function.

We have given here a clear example that a spin liquid GS can be stable in 2D, and yet satisfying all the known constraints given by the LSM theorem. Indeed, spontaneous broken translation symmetry is obtained for any odd number of chains, a remarkable feature since before projection the wave function is translational invariant. As the number of chains increases the chiral spin liquid appears only in 2D systems, where the spin-Peierls dimer order parameter converges to zero, and no broken translation symmetry is implied in the thermodynamic limit.

The chiral spin-liquid described by the $p$-BCS wave function is also consistent with a recent extension of the LSM to 2D systems with finite aspect ratio $L_y/L_x$. In this case, as pointed out by Oshikawa, the state $|\psi_0\rangle = \hat{O}_{LSM}|\psi_0\rangle$, is not necessarily degenerate with the starting wave function $|\psi_0\rangle$, as in the usual LSM construction. However, through a well-defined adiabatic evolution – in analogy with Laughlin’s treatment of the quantum Hall effect – one can obtain a different state $|\tilde{\psi}_0\rangle$, with the same spatial quantum numbers of $|\psi_0\rangle$ and degenerate with $|\psi_0\rangle$. If $|\psi_0\rangle$ is described by a $p$-BCS state $|\psi_0\rangle$, it is easy, by a small change of the pairing function of the state $|\psi_0\rangle$, i.e., $f_\parallel \to f_\perp$, to define a state $|\tilde{\psi}_0\rangle$ with the same momentum implied by LSM theorem but expected to be degenerate with $|\psi_0\rangle$. In fact, the wave function $|\tilde{\psi}_0\rangle$ can be obtained with the same BCS Hamiltonian $\hat{H}_{pBCS}$ with APBC in the $x$ direction. Then, in presence of a finite gap in the excitation spectrum $\Delta_{BCS} > 0$, the wave functions $|\psi_0\rangle$ and $|\tilde{\psi}_0\rangle$ have the same value on any physical operator, and in particular the Hamiltonian, so that the considered states are degenerate in the thermodynamic limit. This is shown, for instance in Fig. 4a) for the nearest-neighbor total energy contribution.

The state $|\tilde{\psi}_0\rangle$, obtained by the adiabatic evolution of the LSM excitation, $|\tilde{\psi}_0\rangle = \hat{O}_{LSM}|\psi_0\rangle$, is no longer connected to $|\psi_0\rangle$ by any physical operator, and, therefore, no spontaneous dimerization is implied in the thermodynamic limit. Indeed, as shown in Fig. 4b), also in geometries with non-zero aspect ratio the $p$-BCS wave
function has a finite dimer correlation length. We have therefore shown a clear counter example to the so-called Oshikawa conjecture \[10\] that no spin liquid is possible in two or higher dimensions. For the Hamiltonians having the wave function \[10\] as the unique GS, \[15\] the above argumentations are clear cut and conclusive.

In general, projected wave functions of the type \[10\], with a finite gap \(\Delta_{BCS} > 0\), do not necessarily break time reversal, like, for instance, by using a chemical potential outside the band, \[11\] \(d + is\) symmetry, \[12\] or more simply \(s\) symmetry. For all these wave functions we expect a finite dimer order parameter in lattices with infinite aspect ratio in agreement with the LSM theorem.

The finite dimer correlation length represents a remarkable property of this projected chiral BCS wave function. For instance, the conventional short-range RVB \[17\], displays instead power-law dimer correlations in 2D, \[18\] and therefore gapless features which may describe a singular point rather than a 2D spin-liquid phase. The fundamental difference between our chiral RVB and the short-range one is due to the violation of the Marshall sign rule in the former case. This property is observed numerically and may fit well with the present experimental resolutions in High temperature superconductors. \[20\]

In conclusion we have presented a clear example that a spin liquid GS with a gap to all physical excitations, though being with single electron per unit cell, can be realized without violating the LSM theorem and its generalizations in 2D. \[19\]. Our results provide a clear support to the possibility of a true Mott insulator at zero temperature, an insulator that cannot be adiabatically continued to any band insulator, showing that the effect of correlation maybe highly non trivial in 2D systems.

One of us (S.S.) thanks R. Laughlin for many useful discussions and for particularly exciting comments. Thanks to D.J. Scalapino for useful discussions, and for his kind hospitality at UCSB (S.S.). This work was substantially supported by INFN-PRA-MALODI, and partially by MIUR-COFIN 01. L.C. was supported by NSF under grant 000000000.

---

**Table 1:**

| Reference | Details |
|-----------|---------|
| [1] | P.W. Anderson, Mater. Res. Bull 8, 153 (1973). |
| [2] | C.K. Majumdar and D.K. Gosh, J. Math. Phys. 10, 1388 (1969); ibidem 10, 1399 (1969). |
| [3] | S.R. White and I. Affleck, Phys. Rev. B 54, 9862 (1996). |
| [4] | E. Dagotto and T.M. Rice, Science 271, 618 (1996) and references therein. |
| [5] | E.H. Lieb, T.D. Schultz, D.C. Mattis, Ann. Phys. (N.Y.) 16, 407 (1961); I. Affleck and E.H. Lieb, Lett. Math. Phys. 12, 57 (1986). |
| [6] | I. Affleck, Phys. Rev. B 37, 5186 (1988). |
| [7] | M. Oshikawa, Phys. Rev. Lett. 84, 1535 (2000); see also the discussion in G. Misguich et al., Eur. Phys. J. B 26, 167 (2002). |
| [8] | P.W. Anderson, Science 235, 1196 (1987). |
| [9] | L. Capriotti, F. Becca, A. Parola, and S. Sorella, Phys. Rev. Lett. 87, 097201 (2001). |
| [10] | D.A. Ivanov and T. Senthil, Phys. Rev. B 66, 115111 (2002). |
| [11] | A. Paramekanti, M. Randeria, and N. Trivedi, e. print cond-mat/0303360. |
| [12] | X.G. Wen, Phys. Rev. B 44, 2664 (1991). |
| [13] | X.G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B 39, 11413 (1989). |
| [14] | W. Kalleyer and R.B. Laughlin, Phys. Rev. Lett. 59, 2095 (1987); Phys. Rev. B 39, 11879 (1988). |
| [15] | S. Sorella, cond-mat/0201388 lecture notes for the Euro-Winter School Kerkade-NL (2002). |
| [16] | L. Capriotti, F. Becca, A. Parola, and S. Sorella, Phys. Rev. B 67, 212402 (2003). |
| [17] | N. Read and B. Chakraborty, 40, 7133 (1989); N.E. Bonesteel, Phys. Rev. B 40, 8954 (1989). |
| [18] | M.E. Fisher and J. Stephenson, Phys. Rev. 132, 1441 |
(1963).

[19] A.W. Sandvik et al., Phys. Rev. Lett. 89, 247201 (2002).

[20] A. Kaminski et al., Nature 416, 610 (2002).