# Chiral Spin Liquid Wave Function and the Lieb-Schultz-Mattis Theorem

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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 an even number of chains there is no dimerization. The two-dimensional thermodynamic limit is consistently reached for a 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.

A long time after its first proposal [1], 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 [2–4], display a gap to the spin excitations only when a broken translation symmetry is found in GS (e.g., in spin-Peierls systems [2,3]) or when the unit cell contains an even number of spin $1/2$ electrons (e.g., in the two-chain Heisenberg model [4]). 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 [5], whose range of validity has been extended to more interesting 2D cases [6,7].

Recently, there has been an intense theoretical and numerical investigation of nonmagnetic wave functions obtained after Gutzwiller projection of the GS of a BCS Hamiltonian [8–11]. On a rectangular $L_x \times L_y$ lattice, this state can be written in the following general form:

$$|p\text{-BCS}\rangle = \hat{P}_G \left[ \sum_k f_k \hat{c}_{k,\uparrow}^\dagger \hat{c}_{-k,\downarrow}^\dagger \right]^{N/2} |0\rangle, \qquad (1)$$

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 $\hat{c}_{k,\uparrow}^\dagger$ and $\hat{c}_{k,\downarrow}^\dagger$ 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 (1) corresponds to PBC on the spin Hamiltonian, regardless of the choice of boundary con-

ditions 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 (BCSH) [9], 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 [9], and $E_k = \sqrt{|\Delta_k|^2 + \epsilon_k^2}$ represents the spin-half excitation energies of the BCSH.

As clearly pointed out by Wen [12], in the presence of a finite gap $\Delta_{\text{BCS}}$ in the thermodynamic limit, such that $E_k \geq \Delta_{\text{BCS}} > 0$, the corresponding BCS finite correlation length is expected to be robust under Gutzwiller projection. Here, we restrict to this class of nonmagnetic states, considering the projected BCS ($p$-BCS) state which is obtained by a $d + id$ gap function of the form

$$\Delta_k = \Delta_{x^2-y^2}(\cos k_x - \cos k_y) + i\Delta_{xy} \sin k_x \sin k_y. \qquad (2)$$

In the following, we will consider the case of $\Delta_{x^2-y^2} = 2$ and $\Delta_{xy} = 1$. This wave function breaks the time reversal symmetry $\hat{T}$ and the parity symmetry ($x \leftrightarrow y$ in 2D) $\hat{P}$, 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 *chiral* order parameter [13]:

$$\hat{O}_C = \frac{1}{N} \sum_i \hat{\mathbf{S}}_i \cdot (\hat{\mathbf{S}}_{i+d_x} \times \hat{\mathbf{S}}_{i+d_y}), \qquad (3)$$

with $d_x = (1, 0)$ and $d_y = (0, 1)$. Chiral spin liquids were introduced a long time ago [13,14]; however, to our knowledge, this is the first attempt to represent this class of states in the $p$-BCS framework. In finite-size systems, it is convenient to define a wave function which satisfies all the lattice symmetries, including parity. This can be done by suitably choosing the overall phase of the complex wave function (1) and taking its real part. In this case, a spontaneously broken lattice symmetry can occur only in the thermodynamic limit.

In the following, by using a variational Monte Carlo approach, we consider in more detail the relation of the $p$-BCS wave functions with the LSM theorem. Given a short-range spin Hamiltonian $\hat{H}$, 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, $|\psi_0'\rangle = \hat{O}_{\text{LSM}}|\psi_0\rangle$, by means of the LSM operator:

$$\hat{O}_{\text{LSM}} = \exp\left[ i\sum_r \frac{2\pi x}{L_x} \hat{S}_r^z \right], \qquad (4)$$

where $r = (x, y)$ indicates the position of each site on the lattice. The new variational state $|\psi_0'\rangle$ has the following properties: (i) its energy expectation value differs at most by $O(L_y/L_x)$ from the variational energy of $|\psi_0\rangle$ and (ii) 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, $\langle\psi_0'|\psi_0\rangle = 0$ [6].

For a 1D or quasi-1D system with an 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 either a gapless spectrum or, in the 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-Ghosh chain [2]. This result, holding rigorously in the limit of vanishing aspect ratio, has been argued to apply in general for 2D systems [6,7]. 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 $\hat{O}_{\text{LSM}}|p\text{-BCS}\rangle = |p\text{-BCS}'\rangle$, namely, the same type of wave function of Eq. (1) is obtained, with the changes below:

$$k \to \bar{k}, \qquad (5)$$

$$f_k \to \bar{f}_{\bar{k}} = f_{\bar{k}-(\pi/L_x,0)} = f_k, \qquad (6)$$

where the new quantized momenta $\bar{k} = k + (\pi/L_x, 0)$ are obtained by interchanging PBC with APBC in the $x$ direction only and Eq. (6) means that the pairing function is calculated with the old momenta $k$: $f_k \hat{c}_{\bar{k}\uparrow}^\dagger \hat{c}_{-\bar{k}\downarrow}^\dagger$. By definition, the wave function $|p\text{-BCS}'\rangle$ has therefore the same quantum numbers predicted by the LSM theorem, the change of momentum being implied by Eq. (5). The reason why the momentum of the wave function (1) can be nonzero for an 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 $|p\text{-BCS}'\rangle$ 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 an odd number of chains. Analogously, the excitations obtained by modifying only the boundary conditions in the BCSH (in the $x$ and/or $y$ direction), namely, using Eq. (5) (and/or its equivalent for the $y$ direction) and $f_k \to f_{\bar{k}}$, may display in 2D the topological degeneracy of this spin liquid wave function [10,11].

We now assume that the $p$-BCS wave function (1) with $\Delta_k$ given by Eq. (2) represents the GS of some short-range Hamiltonian. Certainly, explicit Hamiltonians with short-range off-diagonal matrix elements can be constructed by a simple inversion scheme [15]. This can be obtained considering a given basis of configurations $\{|x\rangle\}$, where the positions and the spins of the electrons are defined. First, we expand the wave function (1) in this local basis as $|p\text{-BCS}\rangle = \sum_x \phi_x |x\rangle$. Then, starting from a local and short-range Hamiltonian $\hat{H}$ with matrix elements $H_{x,x'}$ (e.g., a frustrated Heisenberg model), it is possible to define an effective Hamiltonian $\hat{H}^{\text{eff}}$ by modifying the matrix elements as follows:

$$H_{x',x}^{\text{eff}} = \begin{cases} \mathcal{V}^{\text{eff}}(x) & \text{for } x' = x \\ H_{x',x} & \text{if } s_{x',x} < 0 \\ 0 & \text{if } s_{x',x} > 0, \end{cases} \qquad (7)$$

where $s_{x',x} = \phi_{x'} H_{x',x} \phi_x$ for $x' \neq x$ and $s_{x,x} = 0$, and the diagonal potential is given by $\mathcal{V}^{\text{eff}}(x) = -\sum_{x', s_{x',x}<0} \phi_{x'} H_{x',x}/\phi_x$. It is easily verified that $|p\text{-BCS}\rangle$ is an eigenstate of $\hat{H}^{\text{eff}}$, as $\hat{H}^{\text{eff}}|p\text{-BCS}\rangle = 0$. Then, if $\hat{U}$ is a unitary transformation such that $|x\rangle \to \text{sign}(\phi_x)|x\rangle$, $\hat{U}^\dagger|p\text{-BCS}\rangle$ has all positive coefficients and the transformed Hamiltonian $\hat{U}^\dagger \hat{H}^{\text{eff}} \hat{U}$ has all nonpositive off-diagonal matrix elements. Therefore, due to the Perron-Frobenius theorem, $|p\text{-BCS}\rangle$ is the GS of $\hat{H}^{\text{eff}}$. It is worth noting that, since the LSM operator $\hat{O}_{\text{LSM}}$ is diagonal in the chosen basis, it is straightforward to show that the LSM theorem holds for the effective Hamiltonian (7).

Besides the fact of being the GS of the effective Hamiltonian (7), the complex $|p\text{-BCS}\rangle$ is also a very good variational state for simple frustrated systems, e.g., the so-called $J_1 - J_2$ model in the gapped region ($J_2/J_1 \simeq 0.5$). Indeed, having a finite gap $\Delta_{\text{BCS}}$, the $|p\text{-BCS}\rangle$ wave function describes a spin system with a finite correlation length, and, consequently, a finite triplet gap. For this type of Hamiltonian, the most relevant order parameter in the nonmagnetic phases is known to be the dimer one [16]. Hence, we focus our attention on the dimer-dimer correlations on each chain, $\Delta(r - r') = \langle \hat{S}_r^z \hat{S}_{r+d_x}^z \hat{S}_{r'}^z \hat{S}_{r'+d_x}^z \rangle$, which behaves for large distance as
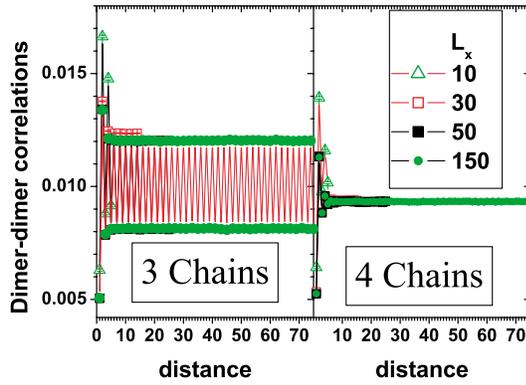
FIG. 1 (color online). Dimer-dimer correlation functions as a function of the distance for three and four chains with PBC on both directions.



FIG. 2 (color online). (left panel) Finite-size scaling of the dimer order parameter in the rectangular geometries with an odd number of chains. ( right panel) Dimer order parameter as a function of the number of chains. The full circles in the right panel refer to the short-range resonating valence bond state, defined as the superposition of all nearest-neighbor dimer coverings of the lattice with the same weights, having $\xi \rightarrow \infty$ in 2D.

$(-1)^{(x-x')} O_{SP}^2/36 + \text{const}$, being $O_{SP}$ the dimer order parameter [3]. As shown in Fig. 1 for the three-chain case, spontaneous dimerization is obtained in the thermodynamic system for odd-leg ladders. Here, in strong analogy with the one-dimensional Heisenberg model in the gapped phase [2,3], the broken translation symmetry allows the system to satisfy the LSM theorem. In contrast, on any even-leg ladder, the $p$-BCS state does not break translational invariance, as shown in Fig. 1 for the four-chain system. Despite the dichotomy between the odd- and even-leg cases, the 2D thermodynamic limit can be still consistently defined. In fact, as it is clearly shown in Fig. 2, though a finite dimer order parameter is obtained for any odd-leg ladder, the order parameter is *exponentially* decreasing with the number of chains. 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 [17]. Indeed, no simple (two-spin) local operator connects the degenerate states in 2D. Moreover, the matrix element of the most relevant 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 the order parameter (see Fig. 2). No other order is detected by studying dimer correlations. Remarkably, by studying the chiral-chiral correlations at the maximum distance along the leg direction, it is possible to show that the chiral order parameter $O_C$ remains a genuine feature of this variational wave function even in the 2D limit [see Fig. 3(a)].

We have given here a clear example that a spin liquid GS can be stable in 2D, 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 translationally 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 $L_y/L_x$ [7]. 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 (1), by a small change
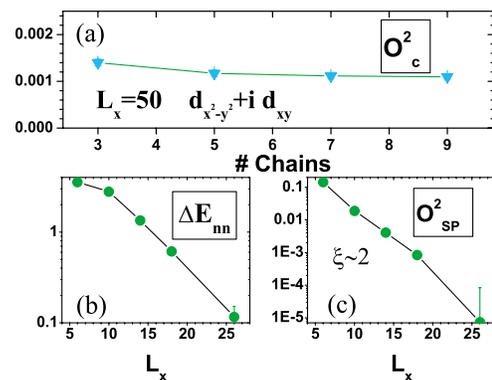


FIG. 3 (color online). (a) Chiral order parameter as a function of the number of chains. (b) Difference of the nearest-neighbor total energy $\Delta E_{nn} = N[\langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle_e - \langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle_o]$ between two orthogonal states $|e\rangle$ and $|o\rangle$ predicted by the LSM theorem. (c) Finite-size scaling of the dimer order parameter in rectangular lattices with finite aspect ratio. For (b) and (c), $L_y = L_x + 1$.

of the pairing function of the state $|\psi_0'\rangle$, i.e., $\bar{f}_{\bar{k}} \to f_{\bar{k}}$, it is easy to define a state $|\tilde{\psi}_0'\rangle$ with the same momentum implied by the 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* BCSH with APBC in the $x$ direction. Then, in the presence of a finite gap in the excitation spectrum $\Delta_{\mathrm{BCS}} > 0$, the wave functions $|\psi_0\rangle$ and $|\tilde{\psi}_0'\rangle$ have the same value of any physical, i.e., local, operator, and, in particular, the Hamiltonian, so that the considered states are degenerate in the thermodynamic limit. In particular, the difference of the nearest-neighbor total energy of the two states is vanishing *exponentially* with the number of chains [see Fig. 3(b)].

The state $|\tilde{\psi}_0'\rangle$, obtained by the adiabatic evolution of the LSM excitation, $|\psi_0'\rangle = \hat{O}_{\mathrm{LSM}}|\psi_0\rangle$, 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. 3(c), also in geometries with nonzero aspect ratio the $p$-BCS wave function has a finite dimer correlation length. We have therefore shown a clear counterexample to the so-called Oshikawa conjecture [7] that no spin liquid is possible for a spin one-half model in two or higher dimensions.

In general, projected wave functions of the type (1) with a finite gap $\Delta_{\mathrm{BCS}} > 0$ do not necessarily break time reversal. For instance, a gapped BCS spectrum can be obtained with a chemical potential outside the band [11], with a gap function with $d + is$ symmetry [12], or simply with $s$ symmetry. For all these wave functions, a finite dimer order parameter, in some cases very small but always nonzero, is found in lattices with infinite aspect ratio, in agreement with the LSM theorem. Therefore, we believe that the broken time reversal is not a necessary condition to satisfy the LSM theorem.

The finite dimer correlation length represents a remarkable property of the chiral $p$-BCS wave function. For instance, the conventional short-range resonating valence bond (RVB) [18] displays instead power-law dimer correlations in 2D [19], 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, for instance, in the GS of the $J_1 - J_2$ model in the strongly frustrated region $J_2/J_1 \simeq 0.5$, where this complex wave function has a lower variational energy compared with the real ones [9]. Thus, we expect that a true spin liquid phase cannot be stabilized in the spin models where the wave function signs are not allowed to change as a function of the parameters of the Hamiltonian [20]. The complex wave function with $d$-wave symmetry proposed here appears to be a reasonable way to open a gap close to a gapless antiferromagnetic phase in a translationally invariant spin model violating the Marshall sign rule, i.e., a *generic* frustrated

model on the square lattice. In this case, the chiral order parameter can be very small, vanishing for $\Delta_{xy} \to 0$ when the correlation length $\xi \to \infty$.

In conclusion, we have presented a clear example that a spin liquid GS with a gap to all physical excitations, though being with one electron per unit cell, can be realized without violating the LSM theorem and its generalizations in 2D. Our results provide a clear support to the possibility of a true Mott insulator at zero temperature, showing that the effect of correlation may be highly nontrivial in 2D systems.

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