Resonating-valence-bond structure of Gutzwiller-projected superconducting wave functions

D. A. Ivanov
Institute of Theoretical Physics, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

Gutzwiller-projected (GP) wave functions have been widely used for describing spin-liquid physics in frustrated magnets and in high-temperature superconductors. Such wave functions are known to represent states of the resonating-valence-bond (RVB) type. In the present work I discuss the RVB structure of a GP singlet superconducting state with nodes in the spectrum. The resulting state for the undoped spin system may be described in terms of the “path integral” over loop coverings of the lattice, thus extending the known construction for RVB states. The problem of topological order in GP states may be reformulated in terms of the statistical behavior of loops. The simple example of the projected $d$-wave state on the square lattice demonstrates that the statistical behavior of loops is renormalized in a nontrivial manner by the projection.

Gutzwiller-projected (GP) wave functions have been often applied to describe the unconventional properties of high-temperature superconductors and the spin-liquid phase of frustrated spin-1/2 systems [1, 2, 3, 4]. Since the early days of their use for strongly correlated systems, GP wave functions have been known not only to provide a good variational ansatz, but also to represent the resonating-valence-bond (RVB) physics of the ground state. Because of their RVB structure, the GP wave functions merit deep investigation as independent objects, irrespective of the underlying physical Hamiltonian [5, 6].

It was shown in the original analysis of GP superconducting wave functions [1] that such wave functions correspond to the RVB states with singlet amplitudes $a_{ij}$ given by the Fourier transform of

$$a(k) = \frac{u_k}{v_k}, \quad (1)$$

where $u_k$ and $v_k$ are the coherence factors of the BCS wave function before projection. For a fully gapped superconductor, this procedure produces amplitudes $a_{ij}$ decaying exponentially with the site separation $|i - j|$, and the interpretation as a RVB state is straightforward. However, in the case of a BCS superconductor with nodes, including the commonly used $d_{x^2-y^2}$ state, this simple derivation produces values of $a(k)$ singular at the nodal points, and the resulting singlet amplitudes $a_{ij}$ are long-ranged. Therefore, in the case of a superconductor with nodes, the conventional derivation cannot interpret the GP wave function as a RVB state.

In this note I resolve the problem of interpreting the physical content of the GP wave function by using an alternative representation in terms of the “loop-soup” path integral. In this construction, well-known for RVB states, the correlation functions are expressed as sums over all close-packed coverings of the lattice with closed loops [6, 8, 9, 10]. In the conventional RVB loop construction, the statistical weights are determined by the products of singlet amplitudes along the loops. In my generalized derivation, the product of singlet amplitudes is replaced by the trace of the product of the BCS Green’s functions along the loop. Thus the role of the RVB singlet amplitudes is played by the BCS Green’s functions $2 \times 2$ matrices. In the case of a superconductor with nodes, the BCS Green’s functions are only marginally local: they decay algebraically with distance. It is therefore clear that caution is required when applying the spin-liquid RVB scenario to high-temperature superconductors [10].

The paper is continued with a brief discussion of the relation of the loop-soup construction to the topological order predicted for RVB states [5, 6, 11, 12, 13]. The presence of topological order corresponds to disordered short-ranged loops.

I then employ the example of the undoped GP $d$-wave state on the square lattice to demonstrate the possibility of strong renormalization of the loop statistics by projection. The loop-length distribution may be characterized by spin-spin correlations which decay algebraically with distance. The power of the algebraic decay is non-universal and depends on the variational parameter of the wave function.

The derivation begins by defining the GP wave function. I consider a system consisting of spins 1/2 occupying a finite lattice with an even number of sites $N$. The GP wave function is constructed by using an auxiliary Hamiltonian of the BCS form,

$$H = \sum_{\{ij\}, \alpha} \left[ t_{ij} \psi_i^\dagger \psi_j \alpha + h.c. \right]$$

$$+ \sum_{\{ij\}} \left[ \Delta_{ij} (\psi_i^\dagger \psi_j^T - \psi_i^T \psi_j^\dagger) + h.c. \right] \quad (2)$$

(in this general form the hopping and pairing amplitudes between any pairs of sites are arbitrary). The Hamiltonian is spin-rotation invariant (it involves only singlet pairing), and its ground state $\Psi_{\text{BCS}}$ is a spin singlet. The GP wave function $\Psi_{\text{GP}}$ for the undoped system is constructed by projecting onto states with exactly one fermion per lattice site (Gutzwiller projection). The resulting wave function may be written as a wave function of spin variables $\Psi_{\text{GP}}(\{\sigma_i\})$, where the spins $\sigma_i$ must contain $N/2$ up and $N/2$ down spins.
The Hamiltonian \( H \) contains more information than required for the construction of the wave function. First, the Gutzwiller projection selects states invariant with respect to SU(2) gauge rotations in the particle-hole space \( \mathbf{14} [16] \). Different Hamiltonians related by such SU(2) gauge symmetries therefore produce the same projected wave function \( \Psi_{\text{GP}} \). Second, the Hamiltonian \( H \) contains information not only about its eigenfunctions, but also about the spectrum, which is not used in the construction of the wavefunction. To eliminate the latter redundancy, we shall use the equal-time Green’s function (the “projector operator”) instead of the Hamiltonian.

To construct the equal-time Green’s functions, we first define the 2\( N \)-dimensional vector space of fermionic operators

\[
\gamma = \sum_i \left[ u(i) \psi_i^\dagger + v(i) \psi_i \right]
\]  

(3)

(the sum is taken over the \( N \) lattice sites). This space has the Hermitian form defined by the anti-commutator \( \{ \gamma_i, \gamma_j \} \), and the Hamiltonian \( H \) acts in this space as a Hermitian operator. The eigenvalue equations are the Bogoliubov–de Gennes equations

\[
[H, \gamma] = E \gamma.
\]  

(4)

The spectrum of the eigenvalues consists of pairs of opposite energies \( \pm E \): this is the consequence of the spin-rotational invariance of the Hamiltonian \( H \). For each solution \( (u, v) \) with energy \( E \), the pair \( (v^*, -u^*) \) gives a solution with energy \(-E\). Thus there are \( N \) positive-energy solutions and \( N \) negative-energy solutions to Eq. (4).

Next we define the projector onto the negative-energy states,

\[
G = \sum_{E_k < 0} |\gamma_k \rangle \langle \gamma_k|,
\]  

(5)

where \( |\gamma_k \rangle \) are normalized eigenstates [solutions of \( H \)]. The operator \( G \) constructed in this way is a 2\( N \times 2N \) Hermitian matrix which may be considered as a single-particle projector onto the negative-energy states or, equivalently, as the matrix of equal-time Green’s functions. It contains no information about the eigenvalues of \( H \), but only about the eigenfunctions. Thus the projector \( G \) contains less information than the original Hamiltonian, but remains sufficient for constructing the multi-particle ground-state wave function.

In real space, the operator \( G \) may be represented by the set of 2 \( \times \) 2 matrices \( G_{ij} \) for each pair of lattice sites \( (i,j) \). The hermiticity implies

\[
G_{ij}^\dagger = G_{ji}.
\]  

(6)

The SU(2) gauge transformation acts on \( G \) by conjugation

\[
G_{ij} \rightarrow W_i^\dagger G_{ij} W_j,
\]  

(7)

where \( W_i \) are the SU(2) matrices of the gauge transformation.

From the completeness of the basis of all states \( \gamma_k \) and from the \( E \rightarrow -E \) symmetry (i.e. from the spin-rotational invariance), we can derive the following identity for \( G_{ij} \):

\[
G_{ij} + J^\dagger G_{ij}^* J = \delta_{ij} 1,
\]  

(8)

Mathematically, this identity expresses the fact that \( G - \frac{1}{2} I \) belongs to the Lie algebra \( \mathfrak{su}(N) \) (see, for example, Ref. [16]). One may verify that Eq. (8) is invariant with respect to SU(2) gauge rotations.

From the SU(2) invariance of Gutzwiller projection, it follows that the wave function depends only on the SU(2)-gauge-invariant properties of the Green’s functions \( G_{ij} \). For future application, we define the cyclic trace of the Green’s functions

\[
T_{i_1...i_l} = \frac{1}{2} \text{Tr}(G_{i_1i_2} G_{i_2i_3} \ldots G_{i_{l-1}i_l}),
\]  

(9)

which depends on the oriented closed loop \( i_1 i_2 \ldots i_l \). This type of cyclic trace appears below in the loop path integral.

To proceed with the loop construction, we first express the wave function in terms of the negative-energy states \( \gamma_k \) and further develop the loop path integral for ground-state expectation values.

The BCS ground state of the Hamiltonian \( H \) may be expressed as

\[
\Psi_{\text{BCS}} = \prod_{E_k < 0} \gamma_k |\downarrow \ldots \downarrow\rangle,
\]  

(10)

where \( |\downarrow \ldots \downarrow\rangle \) is the state with all lattice sites occupied by down spins, \( |\downarrow \ldots \downarrow\rangle = \prod_i |\psi_i^\downarrow \rangle |0\rangle \), and the operators \( \gamma_k \) are the negative-energy eigenvectors of Eq. (4).

After projecting onto singly-occupied states, this wave function may be shown to yield for the GP wave function

\[
\Psi_{\text{GP}}(\{\sigma_i\}) = \text{Det}_{k,i} [u_k(i)|v_k(i)],
\]  

(11)

where \( [u_k(i)|v_k(i)] \) is the \( N \times N \) matrix whose first \( N/2 \) columns are composed of the coefficients \( u_k(i) \) while the last \( N/2 \) columns involve those of \( v_k(i) \). The index \( k \) refers to all negative-energy states and the index \( i \) to all spin-up sites in the given spin configuration \( \{\sigma_i\} \).

Alternatively, the same wave function may be written in the same form (11), but with the index \( i \) labeling spin-down sites. It follows from the rotation invariance that these two determinants must give the same wave function, to within an overall phase factor.

The expression for the “partition function” \( \langle \Psi | \Psi \rangle \) is obtained by taking for the bra-vector the determinant (11) over the spin-up sites and for the ket-vector the same determinant over the spin-down sites. The product of the
two determinants is then rewritten as the determinant of the product of the two matrices (taking the sum over the index $k$) to yield

$$|\Psi_{GP}(\{\sigma_i\})|^2 = \text{const} \det_i G_{ij},$$

(12)

where $i$ labels spin-up sites and $j$ labels spin-down sites. The matrix $[G_{ij}]$ is the $N \times N$ matrix composed of $2 \times 2$ blocks $G_{ij}$. The constant prefactor does not depend on the spin configuration $\{\sigma_i\}$ and will be omitted in further calculations. The expression (12) is explicitly SU(2) gauge-invariant.

The determinant (12) may be further expanded as a product of non-intersecting loops and summed over all possible spin configurations $\{\sigma_i\}$ to produce the partition function $\langle \Psi | \Psi \rangle$. Brief algebraic manipulations using the symmetry (3) give the loop path integral

$$\langle \Psi | \Psi \rangle = \sum_{\{C_n\}} \prod_{n} (-2T_{i_1...i_n}),$$

(13)

where the sum is taken over all coverings by non-intersecting loops of even length, and $T_{i_1...i_n}$ are the loop traces defined in Eq. (4), see Fig. 1. The sum (13) [and all loop sums below] is to be understood as that over oriented loops. From the symmetry (3) it follows that the traces $T_{i_1...i_n}$ for even-length loops are purely real and do not depend on the orientation of the loop. However, it is important to preserve loop orientations in the definition of the sum (13), because they affect the multiplicities of length-two loops: every length-two loop has only one orientation and appears in the sum (13) once; all longer loops admit two orientations and appear twice.

This result has the form of a path integral in which different correlation functions may be computed. For example, the spin-spin correlation function $\langle S_z(i)S_z(j) \rangle$ may be written as

$$\langle S_z(i)S_z(j) \rangle = \frac{1}{\langle \Psi | \Psi \rangle} \sum_{\{C_n\}} (-1)^{P_{ij}} \prod_{n} (-2T_{i_1...i_n}),$$

(14)

where the sum is now taken only over loop coverings with the sites $i$ and $j$ belonging to the same loop, and $(-1)^{P_{ij}}$ takes values $\pm 1$ depending on whether the number of loop links between $i$ and $j$ is even or odd.

The path integral (13) has the same form as the loop construction for RVB states. Most generally, the loop path integral may be written as

$$\langle \Psi | \Psi \rangle = \sum_{\{C_n\}} \prod_{n} A(C_n),$$

(15)

where $A(C_n)$ is an amplitude depending on the geometry of the loop $C_n$.

This general formulation includes many different RVB-type wave functions in a variety of systems. The GP wave functions in Anderson’s derivation [1] correspond to the loop amplitude

$$A(C_n) = -2a_{i_1i_2}a_{i_2i_3}...a_{i_3i_1},$$

(16)

where $a_{ij}$ are the singlet amplitudes defined from (1). Note the importance of the negative sign in the loop amplitudes (13) and (16). This sign arises from the fermionic statistics involved in the GP construction. Alternatively, for a spin system it is possible to construct a “bosonic” product of singlets which leads to a loop amplitude similar to Eq. (16), but without the negative sign [7,13].

Remarkably, the Rokhsar–Kivelson ground state of dimer models [11] may also be described with the same formalism [15]: it is sufficient to set $A(C_n)$ equal to 1 for length-two loops on allowed dimer positions and to 0 otherwise.

The concept of the “loop soup” aids in visualizing the conditions required for the topological order proposed for RVB states [11,12,13]. As explained in Refs. [1,2,14], the different topological sectors on a multiply connected domain (e.g. on a cylinder or a torus) may be accessed by imposing periodic or antiperiodic boundary conditions on the fermions in the Hamiltonian (2) along a topologically nontrivial contour. As a result, the periodic/antiperiodic boundary conditions produce two different GP wave functions $\Psi_+$ and $\Psi_-$. The topological order implies two dual
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jectures.
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the following discussion of those correspondences is not
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conditions (17) may be viewed as an effective absence of in-
bars are of the order of the symbol sizes. The arrow marks
size-dependence of the squared integrated staggered magne-
tem size for any local operator
\[ \langle -1 \rangle^2 \langle \sigma \rangle^2 \propto \phi \]
where the correlation functions must tend to zero suffi-
ciently rapidly (e.g., exponentially) with increasing sys-
t, and involved averaging over \(10^3\) samples. The error bars are smaller than the sym-
\[ \approx \phi \]
It will become clear below that the first of these con-
\[ (\Psi_+|\Psi_-) \rightarrow 0 \],
\[ (\Psi_+|X|\Psi_-) \rightarrow 0 \],
where the correlation functions must tend to zero suffi-
ciently rapidly (e.g., exponentially) with increasing sys-
tem size for any local operator \(X\).

It will become clear below that the first of these conditions \(17\) may be viewed as an effective absence of in-
finite loops in the path integral \(15\), and may be related loosely to the short range of spin correlations. The sec-
ond condition \(18\) corresponds to the absence of valence-
ond crystallization in the RVB construction, and, in the
general case \(15\), may in all probability be formulated as
the absence of loop crystallization. Note, however, that
the following discussion of those correspondences is not
fully rigorous and some statements are indicated as con-
jectures.

I begin by considering the condition \(17\). Under the
assumption that that the Green’s functions \(G_{ij}\) decay
rapidly with distance, loops of large size may appear only

with many links of short length. In this case, the change
of boundary conditions in Eq. \(19\) may be represented by
changing the sign of the Green functions \(G_{ij}\) intersecting
the reference line (Fig. 2). Consequently, the partition
functions in the \(\pm\) sectors may be written as

\[ (\Psi_\pm|X|\Psi_\pm) = \sum_{\{C_n\}} (-1)^W \prod_n (-2T_{i_1...i_n}) \]

where \(W\) is the total winding number of the loops. This
definition may be extended directly to the general for-
malism \(15\) and to any expectation value of a local ob-
servable \(X\),

\[ (\Psi_\pm|X|\Psi_\pm) = \sum_{\{C_n\}} (-1)^W X(\{C_n\}) \prod_n A(C_n) \].

Therefore the difference between the two topological sec-
tors \(17\) contains only configurations with odd winding
numbers. The absence of large loops then serves as a
sufficient condition for the criterion \(17\) of topological
order [I believe that in most situations this is also a ne-
necessary condition]. On the other hand, the absence of
large loops also guarantees that spin correlations \(14\) are
short-ranged, but is not a necessary condition. Therefore
one may expect that in many cases the short range of spin
correlations is related to the condition \(17\), but in this
contribution I provide no rigorous derivation of such a
relation.

We consider next the second condition \(18\). For the
RVB wave functions represented as linear combinations
of products of singlets, this condition corresponds to the
absence of singlet ordering (e.g. the absence of a valence-
ond crystal \(17\)). This can be shown by employing the

FIG. 3: Main panel: staggered spin correlations in the un-
doped projected \(d\)-wave state for different values of the vari-
tional parameter \(\phi = 4 \arctan \Delta\). The Monte Carlo simu-
lation was performed on the \(24\times24\) lattice and involved averaging
over \(10^3\) samples. The error bars are smaller than the sym-

Inset: The exponent \(\alpha\) as defined in Eq. \(23\) as
a function of the variational parameter \(\phi\). Squares: values
of \(\alpha\) obtained from the spatial decay of spin correlations in
the \(24 \times 24\) system. Stars: values of \(\alpha\) obtained from the
size-dependence of the squared integrated staggered magne-
tization \(M(L)\) defined in Eq. \(24\), see Fig. 4 below. The error
bars are of the order of the symbol sizes. The arrow marks
the position of the optimal value of the variational parameter
\(\phi \approx 0.34\pi\) minimizing the variational energy of the Heisen-
berg Hamiltonian within the given class of wave functions
\(10, 24\).

FIG. 4: The dependence of the fluctuating integrated stag-
gered magnetization \(M(L)\) defined in Eq. \(24\) on the linear
system size \(L\) in the log-log scale. The values of \(\alpha\) deduced
from these data are plotted by star symbols in the inset of
Fig. 3.
even-odd basis defined conveniently in the case of RVB or dimer states on a topologically non-trivial domain. Using the expression (20) for the definition of \( \Psi_{\pm} \), the “plus-minus” basis is related to the “even-odd” basis by

\[
\Psi_{\pm} = \Psi_{e} \pm \Psi_{o},
\]

(21)

where \( \Psi_{o} \) and \( \Psi_{e} \) are the states with even and odd numbers of intersections of the singlets (dimers) with the reference line (Fig. 2). The condition (18) may then be reformulated as

\[
\langle \Psi_{e} | X | \Psi_{e} \rangle - \langle \Psi_{o} | X | \Psi_{o} \rangle \to 0
\]

(22)

which, in turn, can be interpreted as the absence of singlet (dimer) crystallization. One may expect that for the more general loop construction (15) this condition also corresponds to the absence of loop crystallization. However, I do not have a rigorous argument supporting this conjecture.

As described above, the first criterion of the topological order involves the question of the effective loop size in the path-integral ensemble. This effective loop size cannot be inferred easily from the singlet amplitudes \( a_{ij} \) (in the case of the RVB construction) or from the Green’s functions \( G_{ij} \). Numerical studies of spin correlations in “bosonic” RVB states indicate that the effective loop size may be renormalized nontrivially by the constraint of fully-packed loops. Similar renormalizations of loop statistics may also be observed in the fermionic GP construction. I consider for illustration one of the simplest examples of a GP wave function, the undoped projected d-wave state on the square lattice. This state has been studied as an approximate ground state of the Heisenberg antiferromagnet. It does not possess long-ranged antiferromagnetic order, but only a power-law decay of antiferromagnetic correlations. The only dimensionless parameter in the wave function is the pairing strength \( \Delta = \Delta/t \), and the wave function is invariant under \( \Delta \to \Delta^{-1} \) (see, for example, Ref. 14). Equivalently, the same wave function may be defined as the projected normal staggered-flux state with a flux per plaquette of \( \phi = 4 \arctan \Delta \). Numerical Monte Carlo simulations indicate that for all values of the parameter \( \phi \), the antiferromagnetic correlations obey the power law,

\[
(-1)^{i-j} \langle S_z(i) S_z(j) \rangle \propto |i - j|^{-\alpha},
\]

(23)

see Fig. 3. One observes that the spin correlations decay very slowly (with \( \alpha < 2 \)), which implies that the effective loop size in the loop path integral (15) is of the order of the system size. The condition (17) of the topological order is therefore expected to fail. Interestingly, in Ref. 2 this state was indeed classified as one without topological order, but on the basis of the failure of the other condition (18) [the condition (17) was not considered for this state]. Note that in the current example (undoped projected d-wave state) the spin correlations probe precisely the probability of the two sites \( i \) and \( j \) belonging to the same loop: the Green’s functions \( G_{ij} \) connect only sites of opposite antiferromagnetic sublattices, and therefore the term \( (-1)^{k_i} \) in (14) is equal to \( (-1)^{i-j} \) independently of the loop configuration.

The actual value of the exponent \( \alpha \) in the power law remains a subject of controversy. One possible scenario is the universal value of \( \alpha \) depending only on the symmetries of the wave function (for example, the authors of Ref. 2 propose the value \( \alpha = 3/2 \)). However, my numerical results suggest a different possibility: a parameter-dependent non-universal exponent \( \alpha(\phi) \). The values \( \alpha(\phi) \) extracted from the spatial decay of spin correlations are shown in the inset of Fig. 3. To verify those results, I have also computed the square of the integrated magnetization in the \( L \times L \) system,

\[
M(L) = \frac{1}{L^2} \left( \sum_{i} (-1)^i S_z(i) \right)^2.
\]

(24)

The dependence of \( M(L) \) on the linear system size \( L \) is plotted in Fig. 3 for three values of \( \phi \). A simple scaling argument predicts \( M(L) \propto L^{2-\alpha} \). The values of \( \alpha(\phi) \) deduced from \( M(L) \) are plotted by star symbols in the inset of Fig. 3. While those results are consistent with a \( \phi \)-dependent value of \( \alpha \), they do not constitute a definite proof: a more detailed analysis of finite-size effects or an analytic argument is needed to settle the issue.

To summarize, the GP superconducting wave functions admit a loop description generalizing the conventional loop construction for RVB states. The role of the singlet amplitudes is played by the equal-time BCS Green’s functions. The properties of topological order and fractionalization are related to the correlations of the loops, but these cannot be inferred simply from the unprojected Green’s functions involved. Nevertheless, the loop formulation may be helpful in visualizing the RVB properties of the GP wave functions, and possibly for developing appropriate analytic approximations.

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