Testing for topological order in variational wavefunctions for $Z_2$ spin liquids

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We determine the conditions under which a spin-liquid Mott insulator $|0\rangle$ defined by a Gutzwiller projected BCS state at half-filling is $Z_2$ fractionalized. We construct a trial vison ($Z_2$ vortex) state $|V\rangle$ by projecting an $hc/2e$ vortex threading the hole of a cylinder/torus and examine its overlap with $|0\rangle$ using analytical and numerical calculations. We find that generically the overlap vanishes in the thermodynamic limit, so the spin-liquid is $Z_2$ fractionalized. We point out the relevance of these results to numerical studies of Hubbard-like models and spin models which have been recently reported to possess spin liquid phases. We also consider possible implications for flux-trapping experiments that have tested for $Z_2$ fractionalization in underdoped high temperature superconductors.

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I. INTRODUCTION

Spin liquid Mott insulators have long been viewed as candidates for the ground state of certain frustrated magnetic systems in dimensions $D \geq 2$. They have been of interest in the context of high temperature superconductivity following Anderson’s proposal2 that doping such insulators may be a novel route to superconductivity. Progress in our theoretical understanding of a certain class of spin liquids has come from two lines of attack over the past decade. First, working from the point of effective theories, it has been shown that spin-liquid insulators in dimensions $D \geq 2$ may emerge as deconfined quantum phases of $Z_2$ gauge theories at zero temperature. In this phase, an $S = 1$ excitation, which is the elementary excitation of a conventional magnet, may break up into two $S = 1/2$ particles, called spinons, which are minimally coupled to an Ising gauge field; hence also the term “$Z_2$ fractionalized spin liquids” for such insulators. The more recent line of progress has been in the construction of simple model Hamiltonians which have no special gauge symmetries but which can nevertheless be shown to possess such $Z_2$ fractionalized phases — these include quantum dimer models on the triangular5 and Kagomé7 lattices, and certain Hubbard-like boson models8,9.

There are a few experimental indications of spin liquid states in two dimensions. Recent low temperature NMR and susceptibility measurements10 in a quasi-2D organic insulator indicate no magnetic phase transitions down to 40mK. Similarly, no ordering transitions are found in Helium-3 adsorbed on graphite11 even at very low temperatures around 10μK. These temperatures are nearly two orders of magnitude smaller than the estimated magnetic exchange energy scale in these respective systems. Further, experimental signatures of spinons have been reported in neutron scattering experiments12 on Cs$_2$CuCl$_4$.

In the past few years, there has also been a lot of numerical work on microscopic models, which are not analytically tractable, searching for spin-liquid phases. In particular, exact diagonalization studies of a multiple-spin exchange model on a triangular lattice13 and Monte Carlo studies of certain two-dimensional Hubbard-like models14,15 indicate that such models may possess, in a regime of parameters, insulating phases with no obvious broken translational or broken spin rotational symmetries.

What kind of spin liquids could these experiments and numerical studies be probing? In order to show how to answer this question in the context of numerical studies, we focus on “topological order” which is a sharp test of whether the phases being accessed in the numerics are $Z_2$ fractionalized spin liquids. Topological order refers to degeneracies in the spectrum of the Hamiltonian which depend on the topology of the manifold on which the system lives. This may be understood as follows: if the system is in the deconfined phase of a $Z_2$ gauge theory, it necessarily implies a novel gapped excitation in the bulk of the system16, namely the Ising vortex of the $Z_2$ gauge field called the “vison”. However, a vison threading noncontractible loops of the manifold, i.e. threading the holes of the cylinder or torus, does not cost any energy in the thermodynamic limit. This leads to a topological degeneracy of the low energy eigenstates17, which may be viewed as states with/without visions threading the holes of the cylinder or torus. In summary, for a $Z_2$ fractionalized spin-liquid insulator we expect a two-fold degeneracy of the low energy spectrum on a cylinder and a four-fold degeneracy on a torus. If indeed the above numerical studies are probing $Z_2$ fractionalized spin-liquid phases, it would be useful to check if they possess topological order consistent with this phase18.

In this paper, we address the following issues: (a) How can one think about the vison in terms of electronic coordinates? (b) Under what conditions is the vison well-defined, leading to $Z_2$-fractionalization and topological degeneracy in spin-liquid insulators? We show how one
may obtain an estimate of the length scale beyond which fractionalization is apparent, consider its implications for the cuprate superconductors, and also point out how one can use the method described here to test for $Z_2$ topological order in other numerical studies of Hubbard-like models, superconductors. Our work builds upon and extends some of the results of Ivanov and Senthil.  

Throughout this paper, we will discuss the above issues in the context of a specific spin-liquid state, namely a Gutzwiller projected d-wave BCS wavefunction on a square lattice. This wavefunction has been shown to provide a remarkably good description of the superconducting state of the high Tc cuprates over a wide range of doping, and the present study was carried out to examine its implications for the undoped insulator and explore connections with phenomenological theories of the cuprates involving $Z_2$ fractionalization. However, our study serves more generally to illustrate the method of identifying $Z_2$ spin-liquid states either using Gutzwiller projected variational wavefunctions, or even other numerical methods as we discuss in Section II.

## II. Constructing the Visor Wavefunction

We begin with a discussion of how to construct a vison wavefunction in terms of microscopic electronic degrees of freedom, which form the basis of the numerical studies. For conceptual clarity, consider first a square lattice of $L^2$ sites “wrapped” into a cylinder along the $\hat{x}$ direction. The spin-liquid ground states $|0\rangle$ of interest to us are given by the Gutzwiller projection of $N$-particle d-wave BCS states at half-filling ($N = L^2$):

$$|0\rangle = \mathcal{P}|\text{BCS}\rangle = \mathcal{P}\left[\sum_{\mathbf{r},\mathbf{r}'\prime} \varphi(\mathbf{r} - \mathbf{r}') \epsilon_{\mathbf{r}}^\dagger \epsilon_{\mathbf{r}'\prime}^\dagger\right]_{N/2}\langle\text{vac}|.$$  

(1)

Here the pair wavefunction is given explicitly by

$$\varphi(\rho) = L^{-2} \sum_{\mathbf{k}} \exp(i \mathbf{k} \cdot \mathbf{r}) / (\xi_k + \sqrt{\xi_k^2 + \Delta_k^2})$$  

(2)

with $\mathbf{k}$'s are chosen consistent with periodic boundary condition (PBC) along $\hat{x}$. The pair wavefunction is parametrized in terms of two variational parameters $\mu$ and $\Delta$ which determine $\xi_k = \epsilon(k) - \mu$, with $\epsilon(k) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$ and $\Delta_k = \Delta(\cos k_x - \cos k_y) / 2$. The Gutzwiller projection operator $\mathcal{P} = \prod_{i}(1 - n_{\uparrow} n_{\downarrow})$ restricts the configurations to have exactly one electron per site.

While the state before projection describes a superconductor, the projected state is an insulator with one electron (or equivalently one spin) per site, and no long range magnetic order.

To test for $Z_2$ fractionalization, we would like to construct a trial state for a vison threading a hole of the cylinder to check for topological order. We do this in two steps. First, we construct a wavefunction for an $hc/2e$ vortex threading the hole of the cylinder. Next, we we Gutzwiller project this $hc/2e$ vortex state and present four arguments for why gives us a good candidate for a vison state.

To construct a superconducting state with one $hc/2e$ vortex threading the hole of the cylinder, we modify the pairing function in the BCS ground state as

$$\varphi(\mathbf{r} - \mathbf{r}') \to \exp[i \mathbf{Q} \cdot (\mathbf{r} + \mathbf{r}') / 2] \varphi_A(\mathbf{r} - \mathbf{r}') \equiv \varphi_A(\mathbf{r} - \mathbf{r}'),$$  

(3)

where $\mathbf{Q} = 2\pi \hat{x} / L$. This gives a center of mass momentum $\mathbf{Q}$ to each Cooper pair and twists the phase of the condensate by $2\pi$ going around the cylinder. However, the requirement of a single-valued wavefunction when even one of the electrons of the Cooper pair ($\mathbf{r}$ or $\mathbf{r}'$) goes around the cylinder, constrains $\mathbf{k}$'s to satisfy antiperiodic boundary conditions (APBC) along $\hat{x}$ in the Fourier transform in defining $\varphi_A(\mathbf{r} - \mathbf{r}')$ via equations analogous to Eqs. 12: hence the subscript $A$ on $\varphi_A(\mathbf{r} - \mathbf{r}')$ in Eq. 3 above. Clearly the state with one $hc/2e$ vortex has a current flow and it can also be written as

$$|hc/2e\rangle_y = \exp\left( i \sum_{\mathbf{r}} \frac{\mathbf{Q} \cdot \mathbf{r}}{2} [n_{\uparrow}(\mathbf{r}) + n_{\downarrow}(\mathbf{r})]\right) \times \left[ \sum_{\mathbf{r},\mathbf{r}'\prime} \varphi_A(\mathbf{r} - \mathbf{r}') \epsilon_{\mathbf{r}}^\dagger \epsilon_{\mathbf{r}'\prime}^\dagger \right]_{N/2}|\text{vac}\rangle.$$  

(4)

Gutzwiller projecting this state at half-filling fixes $n_{\uparrow}(\mathbf{r}) + n_{\downarrow}(\mathbf{r}) = 1$, and the prefactor multiplying the wavefunction in Eq. 4 then drops out as a trivial phase factor since it is independent of the spin configuration. This gives

$$|V_y\rangle \equiv \mathcal{P}|hc/2e\rangle_y = \mathcal{P}\left[\sum_{\mathbf{r},\mathbf{r}'\prime} \varphi_A(\mathbf{r} - \mathbf{r}') \epsilon_{\mathbf{r}}^\dagger \epsilon_{\mathbf{r}'\prime}^\dagger \right]_{N/2}$$  

(5)

Thus the Gutzwiller projected $hc/2e$ vortex state $|V_y\rangle$ simplifies to a form identical to Eq. 1, with $\varphi \to \varphi_A$, and corresponds to imposing antiperiodic boundary conditions on the electrons before projecting them.

Why is this a good candidate for a vison state? First, a projected $hc/e$ vortex with $\mathbf{Q} = 4\pi \hat{x} / L$ does not require any change in BC’s on $\varphi$ to ensure single-valuedness, and the phase factors again drop out at half-filling. It is thus identical to the ground state $|0\rangle$. Hence we only have two kinds of vortex states upon projection: all superconducting states with an even number of $hc/2e$ vortices threading the cylinder collapse onto the ground state $|0\rangle$, those with an odd number of $hc/2e$ vortices threading the cylinder collapse onto $|V_y\rangle$. This renders manifest the $Z_2$ character of a projected $hc/2e$ vortex — two vortices is the same as none — which makes them attractive candidates for visons.

Second, we can look at the crystal momentum of the projected vortex. The vortex state before projection has a crystal momentum $\mathbf{Q}$ per singlet pair, or a total crystal momentum of $\mathbf{Q} N/2$. Since the Gutzwiller projection operator commutes with the translation operator,
the crystal momentum is unchanged by projection. Thus
for a system with dimensions \( L_x \times L_y \), the projected vortex has a total crystal momentum \( P_x = \pi L_y \). Since the crystal momentum is only defined modulo \( 2\pi \), this means the projected \( \hbar c/2\pi \) vortex wavefunction carries momentum \( \pi \) for odd-\( L_y \) and no momentum for even-\( L_y \). As shown elsewhere, this is precisely the momentum of a vison in an insulator described by a \( \mathbb{Z}_2 \) gauge theory with one spin per site. Thus the momentum quantum number of the projected \( \hbar c/2\pi \) vortex is consistent with that of the vison. As discussed below, we will always work with even-\( L_y \) in this paper.

Third, one can consider a specific limit of the pair wavefunction, namely \( \mu \to -\infty \), which corresponds to having singlet pairs only on neighboring sites, like in a nearest neighbor dimer model. The state \( |0\rangle \) corresponds to a superposition of nearest neighbor dimer (singlet) configurations. In this limit, due to the antiperiodic boundary conditions on \( \varphi_A(\mathbf{r} - \mathbf{r}') \), it is straightforward to show that every configuration in which an odd number of singlets lie on links such that one spin of the singlet is at a site \( (L_x, y) \) and the other spin lies at \( (1, y) \) (taking into account all allowed \( y \)) has an amplitude which differs in sign from its amplitude in the state \( |0\rangle \). This is however identical to the well-known construction of the \( \mathbb{Z}_2 \) vison threading a cylinder in the context of dimer models.

Finally, in terms of a dual theory of vortices, the way to obtain a \( \mathbb{Z}_2 \) fractionalized insulator starting from a superconducting state is by condensing pairs of \( \hbar c/2\pi \) vortices, thus quantum disordering the superconductor. In this case, the vison is the remnant of the \( \hbar c/2\pi \) vortex which has not condensed. Since Gutzwiller projecting a superconductor at half-filling fixes the number of particles, it amounts to phase disordering the superconductor, and this also leads one to suspect that the Gutzwiller projected \( \hbar c/2\pi \) vortex is the vison.

Generalizing the above discussion to a torus, \( |0\rangle \) corresponds to PBC along both \( \hat{x} \) and \( \hat{y} \), \( |V_x\rangle \) and \( |V_y\rangle \) correspond to PBC/APBC and \( |V_{x,y}\rangle \) to APBC along both directions. These proposed vortex wavefunctions are designed to investigate the existence of disconnected topological sectors as evidence for fractionalization as we discuss in the following section. A vison excitation in the bulk, on the other hand, would need to have a \( \mathbb{Z}_2 \) flux piercing the plane of the lattice and would require careful consideration of the superconducting vortex core prior to projection, which we avoid here.

III. HOW DO WE TEST FOR TOPOLOGICAL ORDER?

A SC state with a vortex threading the hole of the cylinder/torus carries current and is orthogonal to the ground state. However, Gutzwiller projecting the BCS wavefunction at half-filling destroys SC order and results in an translationally invariant insulator. The key question then is: does any remnant of vorticity survive projection? If it does, then \( \langle V_x |0\rangle = \langle V_y |0\rangle = 0 \) for \( \alpha, \beta = x, y, xy \), the vison is well-defined leading to topological degeneracy, and one is in a \( \mathbb{Z}_2 \) fractionalized phase. If, on the other hand, the proposed vison state has nonzero overlap with the state \( |0\rangle \) in the thermodynamic limit, one is in a conventional unfractonized phase.

Since we have shown above that the vison state on a cylinder with odd-\( L_y \) carries crystal momentum \( \pi \), it is trivially orthogonal to the ground state \( |0\rangle \) even on a finite system. However this by itself does not tell us anything about topological order since if this state becomes degenerate with the ground state it may mix with the ground state in the thermodynamic limit and break translational symmetry — for instance, this is what is known to happen in any gapped phase of an odd number of coupled spin chains (an \( \text{"odd-leg ladder"} \)), as is well-known from an extension of the Lieb-Schultz-Mattis theorem in one dimension. However, in the limit of infinite number of coupled chains, the order parameter in the broken symmetry state may survive leading to a conventional broken symmetry state in two dimensions, or it may vanish leading to a translationally invariant two-dimensional spin liquid. These two possibilities cannot be distinguished by an overlap calculation with odd-\( L_y \).

For purposes of testing for topological order, we are therefore really interested in the case of even-\( L_y \) where the trial vison state carries no crystal momentum, and it is thus not trivially orthogonal to \( |0\rangle \) on finite-size systems. Showing that the overlap between the ground state and the proposed vison state vanishes in the thermodynamic limit on cylinders or torii with even length in each direction is therefore a crucial step in establishing topological order.

IV. “PHASE DIAGRAM” AND SYMMETRIES

To determine the conditions under which the vison survives, it is useful to consider the full parameter space for projected BCS states at half-filling, which is the \( (\mu', \Delta) \) plane with \( t = 1 \) and \( \Delta \) held fixed at some nonzero value in order to describe a RVB liquid of singlet pairs. Studying this general class of states will be useful since one can check if there are states which are not \( \mathbb{Z}_2 \) fractionalized in some regime of parameters, and ask how the transition from a fractionalized regime to an unfractonized regime is reflected in the overlap of the wavefunctions \( \langle V_x |V_y\rangle \).

We use symmetry arguments to show that not all states in this space are distinct upon projection and \( |0(\mu', \mu)\rangle = |0(-\mu', -\mu)\rangle \). In brief, we can change \( \mu' \to -\mu' \), \( \mu \to -\mu \) by a global particle-hole transformation \( c_{\tau\sigma} \to (-1)^{\tau+\sigma} c_{\tau\sigma}^\dagger \) in the wavefunction, also redefining the \( |\text{vac}\rangle \) since empty sites transform into doubly occupied ones. However, with exactly one particle per site such a particle-hole transformation interchanges \( \uparrow \)-spins.
and implying fractionalization in the short range RVB and unshaded half-planes are related by symmetry (\(t' - \mu\)) and coherently, the overlap of two states from different sec-
tions. In particular, the states with a definite “parity” in the dimer model notation correspond to a superposition of the states with and without a vison \(\varphi(r - r')\) is not obviously short-ranged here.

VI. FURTHER ANALYTICAL INSIGHTS

We next focus on the curve \(\mu = \mu_{BCS}(t')\) (see Fig. III A)), where \(\mu_{BCS}\) yields half-filling for the un-projected BCS state in the grand canonical representation (not fixed particle number representation). This unprojected grand canonical state, which we shall denote as \(|BCS\rangle_{GC}\), viewed as the ground state of a BCS Bogoliubov-de Gennes (BdG) Hamiltonian \(H_{BdG}\), is a coherent superposition of number eigenstates sharply peaked at the correct mean density. Working with the grand canonical wavefunction proves convenient since in our discussion below, we will use certain results valid for the BdG Hamiltonian in order to infer properties of its ground state wavefunction. Note that Gutzwiller projecting the grand canonical wavefunction at half-filling also picks out the projector the BCS state into a staggered flux state. Now let us define local \(SU(2)\) gauge transformations \(U\), generated by \(T_j^+ = c_j^\dagger c_{j+1}\), \(T_j^- = c_j c_{j+1}\), \(T_j^Z = \sum_\sigma c_j^\dagger c_{j+1} - 1\), which mix empty and doubly occupied sites as an \(SU(2)\) doublet, but act trivially on the projected subspace with exactly one particle per site. Gutzwiller projection is then equivalent to projection onto the \(SU(2)\) singlet subspace, and we may write any state \(\langle\Phi\rangle = \int dU \langle\Phi|U\rangle\), where the integral is over all group elements \(U_0 = \exp(i \sum_j T_j^Z \cdot \vartheta_j)\). We can thus write

\[
\langle V|0\rangle = \int dU \langle\Phi|U|BCS\rangle_{GC},
\]

which reduces the problem to computing overlaps of un-projected grand canonical states.

For a nonbipartite lattice (e.g., with \(t' \neq 0\)), one cannot gauge away the off-diagonal term in the d-wave BCS-BdG Hamiltonian by any unitary transformation \(UH_{BdG}U^{-1}\), and the ground state of this transformed Hamiltonian, \(U|BCS\rangle_{GC}\), is thus always a SC ground state (or vortex vacuum) for arbitrary \(U\). Then \(\langle\Phi|U|BCS\rangle_{GC} = 0\) for arbitrary \(U\), and thus \(\langle V|0\rangle\) vanishes. Thus nonbipartiteness is a sufficient condition for fractionalization in Gutzwiller projected d-wave states \(\varphi(r - r')\) when \(\mu = \mu_{BCS}\). Note that if one can show this result directly working with the wavefunction \(|BCS\rangle\) in the fixed number representation (rather than \(|BCS\rangle_{GC}\), without appeal to the BdG Hamiltonian, then this result would be valid for general \(\mu\) and not restricted to \(\mu = \mu_{BCS}\). However, we have not found a simple way to show this.

Let us now turn to the bipartite system (in our case \(t' = 0\)), where it is well known that one can gauge away the off-diagonal part of the BdG Hamiltonian (provided it does not break time reversal) and transform the BCS state into a staggered flux state. Now \(\langle\Phi|U|BCS\rangle_{GC}\) is nonzero for some choice \(U\) and one

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cannot use eq. (3) to argue that \langle V|0\rangle vanishes. Note, this is not a proof that the overlap remains nonzero in the thermodynamic limit since one may worry that this particular \(SU(2)\) rotation, which converts the d-wave state to the staggered flux state, has zero measure in the integral and thus still preserve orthogonality. Our numerical results, presented below, however indicate that the overlap does remain nonzero in the thermodynamic limit when \(t' = 0\), so that the wavefunction at this special point does not describe a \(Z_2\) fractionalized state.

VII. OVERLAPS WITHIN PURE \(Z_2\) GAUGE THEORIES

Before proceeding to the numerics, we discuss how \(\langle V|0\rangle\) is expected to scale with system size in an \(L_x \times L_y\) system. For ease of presentation, we consider the system to be defined on a cylinder as shown in Fig. 2 with periodic boundary conditions along \(\hat{x}\). In a unfractionalized phase the overlap between the states with and without a vison threading the hole of the cylinder will remain nonzero in the thermodynamic limit. However, in a fractionalized phase we argue that on the cylinder the overlap should vanish exponentially with \(L_y\). This is easy to see when the matter fields are gapped (e.g., the short-range RVB limit) and may be integrated out to obtain a 2 + 1 dimensional \(Z_2\) gauge theory. Deep in the deconfining phase the overlap between the states with and without a vison threading the hole of the cylinder will remain nonzero in the thermodynamic limit. However, in a fractionalized state.

We will now examine the ground states of this Hamiltonian (on a cylinder) deep in the deconfined phase, which obtains when \(h/K \ll 1\). To begin, let us consider the extreme limit \(h = 0\). In this case we want to set the flux \(\prod_i \sigma^z = 1\) on each plaquette to minimize the energy of \(H_{Z_2}\) in Eq. (7). One ground state in this limit can be achieved by setting \(\sigma^z = 1\) on each link as shown in Fig. 2(A), and acting on this reference state with \(P_{odd}\). Let us call the resulting state \(|v = 0\rangle\). On a cylinder, the system has a second, distinct, eigenstate \(|v = 1\rangle\); this is obtained by gauge projecting the reference state depicted in Fig. 2(B), where a column of horizontal links has \(\sigma^z = -1\) such that this reference state also has zero flux per plaquette. This state \(|v = 1\rangle\) can be alternatively obtained by acting on the first state \(|v = 0\rangle\) with the operator

\[ V^\dagger = \prod_{i \in \text{column}} \sigma^z_{i,i+\hat{x}} \]  

which may be viewed as the operator which creates a \(Z_2\) vortex (vison) through the hole of the cylinder, since it leads to a change in the product of \(\sigma^z\) taken around the circumference of the cylinder from \(+1 \to -1\). We may loosely refer to it as the one-vison state.

Clearly,

\[ \langle v = 0|v = 1\rangle_{h=0} = 0, \]

the overlap between the two states vanishes identically even for a finite-size system. Since \([V^\dagger,H_{Z_2}] = 0\), the state \(|v = 1\rangle\) is an orthogonal eigenstate degenerate with the state \(|v = 0\rangle\). This leads to the two-fold topological degeneracy on a cylinder.

Let us now turn on a small nonzero \(h\), so that we are still deep in the deconfined phase \(h/K \ll 1\), and calculate the perturbative change in each of the two states above.

\[ h\sigma^z \]  

flips the gauge field on a link from \(+1 \to -1\),
on each link, and at small $h/K$ the ground state $|v = 0\rangle_h$ may be built by taking a reference state which is a direct product on all links of the above superposition, and gauge projecting it using $P_{\text{odd}}$. The second ground state $|v = 1\rangle_h$ is obtained by acting with $V^\dagger$ on $|v = 0\rangle_h$. It is straightforward to see that the overlap $\langle v = 0|v = 1\rangle_h$ vanishes for odd-$L_y$ whereas it is nonzero for even $L_y$. (This is consistent with the one-vison state carrying a non-trivial crystal momentum for odd-$L_y$, which we mentioned earlier.) We can estimate by a direct calculation that in fact the overlap for even $L_y$ scales as $\sim (h/K)^{L_y}$ which vanishes exponentially with increasing $L_y$, leading to two orthogonal states in the thermodynamic limit. Since $[V^\dagger,H_{Z2}] = 0$ even for nonzero $h$, this second state is an orthogonal ground state in the thermodynamic limit. We again recover the topological degeneracy, and see that the no-vison and one-vison states have an overlap which vanishes as $\exp(-L_y/\xi)$ for sufficiently large system sizes. Similar results have been obtained in Ref.\cite{34}.

A simple way to understand the above results is as follows. For a two-state system such as a single-particle in a double-well potential with a finite barrier, there is a nonzero amplitude within perturbation theory for a par- ticle localized in one well to be found in the other well due to tunneling across the barrier leading to a nonzero overlap between states where the particle localized in different wells. For a collective coordinate such as the vison, a “string” of length $L_y$, the tunneling between the two states, with the vison localized within the cylinder or outside the cylinder, proceeds through intermediate states where parts of the string lie in the barrier region and the overlap is thus exponentially small in $L_y$.

The behavior of the overlap with gapless matter fields is less well studied though we expect it to further suppress tunneling and lead to a smaller overlap; numerically (see below) we find clear evidence for exponential decay. Note that this decay is very different from the decay we might expect from the overlap of two general unrelated many-body states of a system with fixed density and $L_xL_y$ sites, which would go as $\sim \exp(-\beta L_xL_y)$ for large system sizes.

\section{VIII. Numerical Results}

We finally discuss numerical results for vison overlaps using the variational Monte Carlo method. For computational simplicity\cite{34} we focus on $(V_x|V_y)$. We choose $t = 1$, and fix $\Delta = 1.25$ for all the calculations\cite{34}. The following results are obtained in regimes where we have given analytical arguments above. (i) In the short-range RVB regime we find that the wavefunction is $Z_2$ fractionalized; see Fig.\ref{fig:overlaps}(A) for large negative $\mu$, where the overlap vanishes even on fairly small system sizes. (ii) On the curve $\mu = \mu_{\text{BCS}}$ we find that nonbipartite (i.e., $t' \neq 0$) wavefunctions are fractionalized as evinced by overlaps which vanish with increasing system size (e.g., the curve in Fig.\ref{fig:overlaps}(A) for $\mu = 0$) indicates a state which is not $Z_2$ fractionalized. The lines are fits to the form $a(1 - \tanh((L - \xi^*)/\xi))$, which works well for all parameters studied, and from which we extract $\xi^*$. (C) Exponential asymptotic behavior of the overlap shown on semi-log plot (see text in Section VIII and Section VII for details).

We next evaluate overlaps at $t' = 0.0, -0.25, -0.5$ for $-1.5 \lesssim \mu \lesssim 1.5$ which, as we discuss below, covers the region of interest for possible spin-liquid insulators in the vicinity of high Tc cuprates. We show in Fig.\ref{fig:overlaps} the overlap $\langle V_x|V_y \rangle$ as a function of system size $L$ for a range of $t$ and $\mu$. We find that at small $L$ the overlaps are finite and then cross over on a scale $\xi^*$ to an asymptotic exponential decay $\exp(-2L/\xi)$. This behavior can be simply described by the functional form $\langle V_x|V_y \rangle/L = a(1 - \tanh((L - \xi^*)/\xi))$ which appears to fit the data well\cite{34}. In particular, this form captures the crossover from a constant on small system sizes to an asymptotic exponential form apparent in Fig.\ref{fig:overlaps}(C).

Deep in the fractionalized regime, we can extract both $\xi^*$ and $\xi$ and we find $\xi^* \approx 2\xi$. However, it is hard to access the asymptotic behavior in the region of interest around $(t' = 0, \mu = 0)$, though we can still reliably extract the crossover scale $\xi^*$.

We plot the inverse length scale $1/\xi^*$ for $t' = 0, -0.25, -0.5$ at different $\mu$ in Fig.\ref{fig:1/xx}. For $t' = 0$, we see that $\xi^* \rightarrow \infty$ as $\mu \rightarrow 0$, fully consistent with the finite overlap independent of $L$ on accessible system sizes.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{overlaps.png}
\caption{Size dependence of the overlap $\langle V_x|V_y \rangle(L)$ for $\Delta = 1.25$ with (A) $t' = 0$ and (B) $t' = -1/4$. The different curves correspond to overlaps for different values of $\mu$ as indicated. An overlap vanishing with increasing system size indicates a $Z_2$ fractionalized state, a non-vanishing overlap (e.g., the curve in (A) for $\mu = 0$) indicates a state which is not $Z_2$ fractionalized. The lines are fits to the form $a(1 - \tanh((L - \xi^*)/\xi))$, which works well for all parameters studied, and from which we extract $\xi^*$. (C) Exponential asymptotic behavior of the overlap shown on semi-log plot (see text in Section VII and Section VIII for details).}
\end{figure}
for \((t', \mu) = (0, 0)\) seen in Fig. E(A). It also clear that \(\xi^*\) remains finite everywhere away from the origin though it may become quite large in its vicinity.

Since fractionalization manifests itself at length scales larger than \(\xi^*\), our numerical results strongly suggest that all points in the phase diagram of Fig. H(A) are fractionalized, except for the origin where \(\xi^*\) diverges. \((t', \mu) = (0, 0)\), with its special bipartite symmetry, is an unfractonized "singular point" in the space of spin-liquid insulators that we study. At this point, the wavefunction has a power law decay of spin correlations\(^{19}\)

\[\sim (-1)^{z+y}/|r|^\alpha\]

with a non-trivial \(\alpha \simeq 1.5\), and thus appears to be magnetically critical as well.

**IX. IMPLICATIONS FOR THE CUPRATES**

Now the question arises — what regime in parameter space is relevant for the cuprates? One possibility is that there are no fractionalized states in the vicinity of the observed phases in real materials. An alternative worth exploring in view of the success of RVB wavefunctions in understanding the SC state\(^{12}\), is that we take the insulating limit (hole doping \(x \to 0\) of \(|\Psi|_{BCS}\)). Further, although \(P|BCS\) is not the ground state of the for the half-filled Hubbard model at large-\(U\), and does not have long-range antiferromagnetic order, it is known to be an energetically competitive candidate state.\(^{19,20}\)

Optimizing variational parameters \(\mu, \Delta\) for the large-\(U\) Hubbard model \((U = 12, t' = -1/4)\), we find \(\Delta \simeq 1.25\) while \(-0.3 \leq \mu \lesssim 0.3\) as shown in Fig. H(B). For this region (the shaded ellipse in Fig. H(A)) we conclude from Fig. H(B) that \(\xi^* \gtrsim 25\) lattice spacings.

We now convert this to an estimate of the energy scale \(E_v\) below which fractionalization is apparent. We expect \(E_v = \alpha J/(\xi^*)^z \lesssim \alpha J/\xi^*\) which vanishes at the "singular point" with bipartite symmetry. Here \(J\) is the nearest-neighbor superexchange, \(\alpha \equiv O(1)\) is a dimensionless constant and the dynamical exponent \(z \gtrsim 1\). For \(\alpha = 1\) and \(J = 1200\)K, the estimated \(E_v \lesssim 50\)K. More concretely, proximity to the unfractonalized 'bipartite' point \((t' = 0, \mu = 0)\) can lead to a very small vison gap for fractionalized RVB states. Recently, based on an ingenious proposal of Senthil and Fisher\(^{28}\), a flux trapping experiment\(^{28}\) was carried out to detect the vison in highly underdoped cuprates. However, these experiments did not see the vison, which led to an upper bound on the vison gap \(\lesssim 150\)K. Our estimates are consistent with this bound, and suggest that \(Z_2\) fractionalization, even if present in the cuprates, would likely be apparent only at very low \(T\) and cannot play a role in pseudogap anomalies.

**X. APPLICATION TO NUMERICAL STUDIES OF HUBBARD-LIKE MODELS**

At this stage, we would like to emphasize the most important general outcome of our numerical results which goes beyond the specific conclusions regarding the particular wavefunction we have studied, and how it can be applied to numerical studies of model systems\(^{13,14,15}\) to test for \(Z_2\) fractionalization. If a system is in a zero fractionalized insulating phase, we have shown that the overlap of the wavefunctions with periodic and antiperiodic boundary conditions imposed on the electrons must vanish exponentially as \(\exp(-L/\xi)\) on an \(L \times L\) system. The length scale beyond which fractionalization is apparent, \(\xi^*\), can be deduced from studying the finite size scaling of this overlap. These two results are useful in detecting topological order when the full low lying spectrum of a microscopic Hamiltonian is not accessible so that the topological degeneracies are not obvious even though one can work with large system sizes.

Consider, for example, Lanczos studies which improve upon a definite triad wavefunction for any Hamiltonian using a few Lanczos iterations\(^{31}\), or other Monte Carlo studies\(^{32}\) which also use wavefunctions. Let us imagine working on a cylinder (or torus), and starting with two different wavefunctions which differ in the boundary conditions imposed on the electrons. In a \(Z_2\) spin liquid insulator, this should provide us with the two topologically degenerate ground states. However, if the Hamiltonian has a conventional ground state however, we expect the two resulting states to be identical.

Note that, if one has small system sizes, the two initial states may have a large overlap even in a \(Z_2\) spin liquid, and then would lead to a single ground state. However, on a large enough system, we expect the initial overlap would be exponentially small in a \(Z_2\) spin liquid, so that one may recover the different topological sectors in this manner. Another check, apart from a vanishing overlap...
of the different final states, is that the energy difference between them should vanish with increasing system size. If the spinon excitations are gapped the energy difference is expected to decay exponentially in \( L \), but it would have a power law decay in the presence of gapless spinon excitations.

### XI. CONCLUDING REMARKS

In this paper, we have analyzed the Gutzwiller projected \( d \)-wave BCS state at half-filling, and shown from analytic arguments and numerical results that it generically describes a \( Z_2 \) fractionalized spin liquid except at a special \( \text{‘bipartite’} \) point where the vison is no longer well defined. We have pointed out the significance of this result for the cuprate superconductors. As mentioned in the introduction, there have been many recent examples of spin-liquid states reported in numerical studies of \( SU(2) \) spin models and Hubbard-like models. These models have been identified as having spin liquid ground states based on the fact that the ground states do not appear to possess any simple broken symmetry patterns. The ideas and methods developed in this paper should be applied to these systems. If they are shown to have topological order consistent with that expected for a \( Z_2 \) spin liquid, they may provide us with the first examples of \( Z_2 \) fractionalization in microscopic models with full spin rotational symmetry.

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29. We have checked that the particular projected wavefunction we use has no long-range magnetic or valence bond order and thus describes a translationally invariant spin-liquid.
30. We have checked that local spin correlations are identical
in the thermodynamic limit for states with and without a vison. These states are thus locally identical and differ only in their global (topological) properties.

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37 This value of $\Delta$ was chosen as it is the value which gives the minimum energy for the Hubbard model at half-filling. For more details on this, see Section IX and Ref. 19.

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