Inhomogeneous states and nodal fermions in the SU(2) gauge theory

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We discuss the issue of phase separation in the SU(2) slave boson theory of Wen and Lee of the doped Mott insulator. It is shown that the constraint structure of the theory leads to the interpretation of the holons to have hard-core interactions, which is demonstrated further by studying the empty limit (no electrons). Surprisingly, with hard-core interactions even the empty limit is described well by the slave-boson theory, both as an energy density and with the regard to dynamical properties. The consequences are investigated in the overdoped superconducting regime, where both phase separation and a d + s structure of the order parameter is obtained. This s-wave component is already imminent in the description of the hole in the slave boson theory. The interacting nature of the holons also lead to sound modes in the single-electron propagator. The novel idea of the isospin spiral is introduced, based on the projective symmetry principles of Wen. This isospin spiral explains the coexistence of superconductivity and the Mott insulating state, being the consequence of phase separation.

Secondly, it might be able to explain why nodal fermions survive in the presence of charge inhomogeneities.

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I. INTRODUCTION

A long standing question in the physics of high-$T_c$ superconductivity is how nodal fermions can coexist with stripes, as experiments seem to point out. There is no simple theoretical explanation on the market as to why charge inhomogeneities do not interact strongly with the low-lying degrees of freedom. A possible explanation is that in the high-$T_c$’s, electrons are splintered into spinons and holons. Being different degrees of freedom, it is possible that charge inhomogeneities do not communicate with the fermionic low-lying excitations. Experimental support for such fractionalisation is for example given by photo-emission.

This idea of fractionalisation is incorporated in the slave boson theories, leading to spin liquid states. These spin liquids are states “nearby” the parent Mott insulating states, and carry nodal excitations. The hope is that these spin liquid states are candidates to describe the evolution from the Mott insulator to the d-wave superconductor, in which quasiparticles with d-wave dispersion are extensively proven experimentally.

These slave theories are plagued by one problem, however: they appear not to be able to describe inhomogeneous states, like stripes, let alone that they can explain coexistence of nodal fermions with stripes. The main point of this article is that the SU(2) slave boson theory as developed by Lee and Wen, is able to capture both aspects. This conclusion is based both on the projective symmetry ideas of X.-G. Wen, and on an improvement of the original theory by Wen and Lee.

The first idea is at the root of our proposal of the isospin spiral. Wen showed that for zero doping, the mean field states describing a staggered flux phase (SFP) and the d-wave superconductor (dSC), are physically the same, i.e., they are gauge equivalent. Only for non-zero doping, this equivalence is broken, such that a d-wave state is favoured, mimicking the instability of the SFP against the dSC. Our idea is now that for low doping, an inhomogeneous state is favourable above a homogeneous dSC. This state connects an SFP with no doping smoothly with a charged superconductor. This leads to a picture in which isolating SFP states coexist with dSC states on stripes. The protection of the nodal fermions lies in the fact that for zero doping, both the SFP and dSC carries nodal excitations.

For these inhomogeneous states to exist, it needs to be proven that the SU(2) slave boson theory supports phase separation, which is not proven so far. We show that this phase separation does occur, which is connected to our technical improvement of the original Wen-Lee theory. It is demonstrated that due to the constraint structure of the theory, the charge carrying holons need to have a hard-core interaction, which accounts for phase separation. The predicted compressibility and critical doping are in accord with chemical potential shift measurements. These phase separation tendencies of the SU(2) gauge theory puts the door ajar for more intricate phenomena, like the stripe order that has been observed in experiments.

In turn, this constraint structure turns out to be responsible for an unexpected surprise: the superconducting order parameter needs to be d + s-wave, instead of d. This interferes in an interesting way with the empirical developments in high-$T_c$ superconductivity. There is strong experimental evidence from c-axis tunneling and Raman scattering that in Bi2212 there is an s-wave component in the gap, which is in largeness comparable to our prediction, and grows with doping, also in accord with our prediction. Further, π-phase shift experiments for YBCO point out that the s-wave component therein cannot be fully explained by the orthorombicity of the crystal. As far as we are aware, SU(2) gauge theory, in our formulation, is the only theory explaining these results in at least an elegant way, and is demonstrated to be rooted in the way SU(2) gauge theories describe doping of holes.

It appears that the above experimental findings are largely ignored because all existing mechanism theories predict either a d-wave or an s-wave, and the SU(2)
gauge theory is stand-only with regard to its insistence on a $d + s$-symmetry. In the narrow context of slave-like theories, Ogata and coworkers excluded $d + s$ in the related context of Gutzwiller projected wave function Ansätze.\textsuperscript{28,29}

The organisation of this paper is as follows. In Section \ref{sec:two} we review the $SU(2)$ gauge theory formulation of Wen and Lee, and mention the projective symmetry ideas of Wen. In Section \ref{sec:three} we take a somewhat warped perspective on doping: to fully understand the effects of doping, we consider the empty limit, i.e., the doping $x = 1$. As academic as it might seem, this exercise is very instructive as to the fact that the slave holons should have hard cores, and that the s-wave order parameter is induced by doping. It turns out that the s-wave component is equal to half times the density of dopant holes. We also show that the mean field theory is able to get both the energy and the single-electron propagator right. Furthermore, the mean field theory in the empty limit gives the inspiration for the mean field wave function to be exploited in our analysis for intermediate dopings in the following section.

In that Section \ref{sec:four} we derive a mean field free energy functional for non-zero doping in the grand canonical ensemble, to be able to account for phase separation. The mean field phase diagram is calculated. The phase separation properties of the hard-core holon $SU(2)$ slave theory is further quantified by comparison of the compressibility with experiments on the chemical potential shifts.\textsuperscript{13} The agreement turns out to be very well. Also the node shift, caused by the s-wave admixture, is determined. The hard-core nature of the bosons leads to interesting and experimental falsifiable properties. Namely, the hole condensate leads to phonon modes in the incoherent part.

In the last Section \ref{sec:five} the idea of the isospin spiral is introduced and quantified. We show that the mean field energy of the inhomogeneous state is only a bit above the energy of the homogeneous state. We argue that this should be viewed as an artefact of the $t - J$-model, and not of the isospin spiral state. We also show that the nodal fermions are not that much affected by the charge inhomogeneities as expected. In effect, the gap is very small, leading to only very small Umklapp scattering at the Fermi pockets.

These interesting results form a promising motivation to study $SU(2)$ gauge theory in more realistic models for the cuprates, the more so since it seems to be the only theory on the market predicting a $d + s$-form of the superconducting order parameter. In fact, $SU(2)$ gauge theory forms the bridge between, on the one hand, nodal fermions and spin liquid states, and on the other hand, striped superconductors.

\section{$SU(2)$-SLAVE BOSON FORMULATION OF THE $t - J$-MODEL}

As is widely accepted, the problem of high-temperature superconductivity, is the problem of doping a Mott insulator. The parent compounds of high-$T_c$ are insulating, due to a large Coulomb repulsion. By removing electrons however, the charges get mobile, and it is believed that this physics is at the origin of the superconductivity. This forms the motivation to include the hopping of projected electrons $\tilde{c}_{i\sigma}$ in the original Heisenberg Hamiltonian:

$$H_{t-J} = \sum_{<ij>} J (S_i \cdot S_j - \frac{1}{4} n_i n_j) - \sum_{ij} t_{ij} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + h.c.),$$

where the hoppings $t_{ij}$ are the wave function overlaps of electrons at sites $i$ and $j$. Without loss of generality, we take $t_{ij} = t$ for nearest neighbour sites, and $t_{ij} = 0$ otherwise.

The idea of the $SU(2)$ slave boson formulation, due to Wen and Lee\textsuperscript{12}, is rooted in the observation by Affleck and Marston\textsuperscript{11} that the spin system at half-filling in a fermionic ‘spinon’ representation is characterised by both the usual ‘stay at home’ $U(1)$ gauge symmetry, and a local conjugation symmetry meaning that one can describe the spin system equally well in terms of spinon particles and antiparticles. This idea is encoded in introducing the $SU(2)$ doublet composed from the spinon operators $f_{i\uparrow}$ and $f_{i\downarrow}$.

$$\psi_i = \begin{pmatrix} f_{i\uparrow} \\ f_{i\downarrow} \end{pmatrix}. \quad (2)$$

In this language, the spin operators are given by

$$S^+_{i\uparrow} = \frac{1}{2} (\psi_{i\uparrow} \psi_{2\downarrow}^\dagger - \psi_{2\uparrow} \psi_{i\downarrow}^\dagger) \quad (3)$$
$$S^z_{i\uparrow} = \frac{1}{2} (\psi_{i\uparrow} \psi_{i\downarrow} - 1). \quad (4)$$

Importantly, the Hilbert space of the $t - J$ Hamiltonian is formed from three states only: a spin up electron, $c_{i\uparrow}^\dagger |\text{vac}\rangle$, a spin down electron $c_{i\downarrow}^\dagger |\text{vac}\rangle$ and a vacancy $|\text{vac}\rangle$. Consequently, the electron operators in Eq.(1) are projected electron operators $\tilde{c}_{i\alpha} = c_{i\alpha}(1 - n_{i\bar{\alpha}})$, where $\bar{\alpha}$ denotes a spin opposite from $\alpha$. The tilde is dropped from now on and the projection is kept implicit. Bear in mind that one should take care that all physics takes place in this projected Hilbert space!

Let us now describe these electrons in the $SU(2)$ gauge theory. Since in everyday life only the physical electrons are encountered, the electrons should be $SU(2)$ singlets. To construct these singlets, introduce the $SU(2)$ doublet describing holons:

$$h_i = \begin{pmatrix} b_{i\downarrow} \\ b_{i\uparrow} \end{pmatrix}. \quad (5)$$
Then the appropriate SU(2) singlet describing the projected electron is
\[ c_{\uparrow i} = \frac{1}{\sqrt{2}} h_i^\dagger \psi_i = \frac{1}{\sqrt{2}} (b_{i1}^\dagger f_{1i} + b_{i2}^\dagger f_{1i}), \]
\[ c_{\downarrow i} = \frac{1}{\sqrt{2}} h_i \psi_i = \frac{1}{\sqrt{2}} (b_{i1} f_{1i} - b_{i2} f_{1i}). \]

The equations (6) as they stand, however, are not operator equalities, since the Hilbert space of the SU(2) theory is larger. To arrive at the correct physics, we have to impose constraint to make the mapping to the states of the original t–J-Hamiltonian exact, so that the Hilbert spaces are equal. This is achieved as follows. Since the electrons should be SU(2) singlets, we should require that the physical states |phys⟩ of the SU(2) slave boson model obey
\[ (\psi^\dagger_i \tau^l \psi_i + h_i^\dagger \tau^l h_i) |\text{phys}\rangle = 0. \]

There are precisely three states satisfying Eq. (8). The first two states satisfying those, are \( f_{1i}^\dagger |\text{vac}\rangle \) and \( f_{1i}^\dagger |\text{vac}\rangle \), corresponding the projected up and down electron in the first two states satisfying those, are to the introduction of the holon doublet Eq.(5). This is achieved as follows.

In order to make progress, we are going to put forward a mean field theory, and treat the constraints on a mean field level.

\[ |0\rangle_i = \frac{1}{\sqrt{2}} (b_{i1}^\dagger + b_{i2}^\dagger f_{1i} f_{1i}^\dagger) |\text{vac}\rangle_i. \]

It is easy to check that Eq. (9) does satisfy all the constraints Eq. (8). Observe that we needed all the three constraints to arrive at this expression. In the original Wen and Lee formulation, the consequences of this fact have not been taken at face value. It will be demonstrated that this is not justified for higher dopings.

In the expression for the hole, SU(2) gauge theory already reveals some of its powers: it captures the fact associated with the particle-hole symmetry intrinsic to spin that the singletness of pure vacuum should be treated on precisely the same footing as the spin singletness of either the empty or doubly occupied spinon configuration.

In this way, it is shown how one can make a mapping from the slave boson operator states to the Hilbert space of the t−J model, by including exact constraints Eq.(8). Solving for exact constraints is however extremely difficult.

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one may assume the existence of the fermionic vacuum expectation values
\[ \chi_{ij} = \langle f_{ij}^\dagger f_{ij} + f_{ij} f_{ij}^\dagger \rangle \]
\[ \Delta_{ij} = \langle f_{ij} f_{ij}^\dagger - f_{ij}^\dagger f_{ij} \rangle. \]

The first one is a hopping amplitude, inspired by the staggered flux spin liquid states proposed by Affleck and Marston. The order parameter \( \Delta \) is going to play the role of a superconducting amplitude with d-wave symmetry.

Let us now assume that the expectation values Eq. (10) and Eq. (11) exist, and let us presuppose deconfinement, by neglecting fluctuations in the gauge fields \( a_{ij}^\dagger \).

This is equivalent to replacing of the exact constraints Eq. (8) by the mean field constraints
\[ \langle \psi_i^\dagger \tau^l \psi_i \rangle = 0. \]

Let us first obtain a manifestly invariant SU(2) gauge invariant mean field theory, by grouping the mean fields as follows:
\[ U_{ij} = \left( -\chi_{ij}^\dagger \Delta_{ij} \chi_{ij} \right). \]

To actually calculate matters, we have to derive the slave boson version of the Hamiltonian Eq.(11), with the decomposition Eq.(10). To decouple terms quartic in the spinons, we use the spin liquid Ansatzes Eqs. (10) and (11). In order to impose the three constraints Eq. (29), we need to incorporate the Lagrange multipliers \( a_{ij}^\dagger \) into the mean field Hamiltonian. Bearing these remarks in mind, it is a straightforward exercise to derive the mean field Hamiltonian

\[ H_{mf} = -\mu \sum_i h_i^\dagger h_i - \sum_i a_{ij}^\dagger \left( \frac{1}{2} \chi_{ij}^\dagger \psi_{ij} \psi_{ij} + h_i^\dagger \tau^l h_i \right) + \sum_{<ij>} \frac{3J}{8} \left( |\chi_{ij}|^2 + |\Delta_{ij}|^2 + \psi_{ij}^\dagger U_{ij} \psi_{ij} + h.c. \right) + \sum_{<ij>} t \left( h_i^\dagger U_{ij} h_j + h.c. \right), \]

where \( U_{ij} \) was already defined in Eq.(13).

Of course, the Hamiltonian Eq.(14) is manifestly SU(2) invariant under the transformation
\[ \psi_i \rightarrow g_i \psi_i, \ h_i \rightarrow g_i h_i, \ U_{ij} \rightarrow U_{ij} g_i g_j^\dagger, \ a_{ij}^\dagger \tau^l \rightarrow a_{ij}^\dagger \tau^l = g_i a_{ij}^\dagger \tau^l g_j^\dagger. \]

Inspired by the spin liquid ideas of many people, an idea having some experimental support, we introduce three mean field states, namely the staggered flux phase, the d-wave density wave state and the d-wave superconductor. We recall their descriptions here.

The d-wave superconductor is in the projective symmetry group represented by

\[ \text{dSC} \]
\[ U_{i,1} = -\chi \tau^3 + \Delta \tau^1, \]
\[ U_{i,2} = -\chi \tau^3 - \Delta \tau^1, \]
\[ a_{ij}^\dagger = 0, \ a_{ij}^\dagger a_{ij}^\dagger \neq 0, \]
\[ <b_1> = <b_2> \neq 0. \]
The dispersion for the fermions is (at least for homogeneous \(a_{0i}\)) readily calculated to be
\[
E_k = \sqrt{(\chi_k - a_{0i}^3)^2 + (\Delta_k - a_{0i}^1)^2},
\]
\[
\chi_k = -\frac{3J}{4}(\cos k_x + \cos k_y)\chi,
\]
\[
\Delta_k = -\frac{3J}{4}(\cos k_x - \cos k_y)\Delta.
\]
(17)

One should notice that the spinons have gapless Dirac dispersions at the points \((k_{x}, k_{y}) = (\pm \frac{\pi}{2}, \pm \frac{\pi}{2})\), i.e., at those points we have nodal fermions consistent with experiments.35,36

The following two phases also support these Dirac quasiparticles. The first one is the staggered flux phase, SFP
\[
U_{1i+\hat{x}} = -\chi \tau^3 - i(-)^I \Delta,
\]
\[
U_{1i+\hat{y}} = -\chi \tau^3 + i(-)^I \Delta,
\]
\[
a_{0i}^{1,2,3} = 0,
\]
\[
< b_1 > = < b_2 > = 0.
\]
(18)

The third phase has Fermi pockets, with nodes radially shifted from \((\frac{\pi}{2}, \frac{\pi}{2})\):
\[
dSC with pockets
\]
\[
U_{1i+\hat{x}} = -\chi \tau^3 - i(-)^I \Delta,
\]
\[
U_{1i+\hat{y}} = -\chi \tau^3 + i(-)^I \Delta,
\]
\[
a_{0i}^{1,2} = 0, a_{0i}^3 \neq 0
\]
\[
< b_1 > \neq 0, < b_2 > = 0.
\]
(19)

We remind the reader that the dSC state is referred to that way, since in the Hamiltonian Eq. (14) that particular \(U_{ij}\) couples \(f_{1i}\) with \(f_{1j}\).

The SFP is a spin liquid, describing spinons hopping around the plaquettes of the square copper-oxide lattice. It breaks translation symmetry, since the hopping fluxes
\[
\Phi_{\text{hop}} = \frac{\pi}{4} \sum_{\text{plaquette}} \text{Arg}(U_{ij}^{11}) = \pm \frac{\Delta}{\pi}
\]
show a bipartite staggered pattern. By a Fourier transformation to momentum space, the dispersion is readily calculated. It turns out to be identical to the dSC-dispersion
\[
E_k = \sqrt{(\chi_k - a_{0i}^3)^2 + (\Delta_k - a_{0i}^1)^2},
\]
(21)

The framework of classical Landau-Ginzburg-Wilson theory, this is impossible: in general, different symmetry broken states give rise to different excitations. What is going on here? In fact, the two above states are two sides of the same coin. This is seen after applying the following site-dependent transformation,
\[
g_i = \exp \left(-i \frac{\pi}{4} (-)^I \tau^1 \right)
\]
(22)
by which the SFP is mapped to the dSC. (The quantity \(I\) is defined as \(I = i x + iy\).) Put differently, the translational symmetry breaking of the SFP is just a gauge artefact. Due to the idea of Wen,33 this is an expression of the fact that for zero doping, these states are members of the same projective symmetry group (PSG). This means that different mean field states describing the same physics, are connected to each other by gauge transformations. Wen then declares them to have the same quantum order, a novel concept going beyond the standard Ginzburg-Landau-Wilson paradigm.

In fact, all states connected to the dSC by a gauge transformation
\[
g_i = \exp (-i \theta_i \tau^1)
\]
(23)
are equivalent. This can be pictured nicely by the concept of the isospin sphere. An \(SU(2)\)-gauge group element \(g_i\) can be written as follows:
\[
g_i = \left( \frac{z_{11} - z_{12}^*}{z_{11}}, \frac{z_{12}^*}{z_{11}} \right)
\]
(24)
where the complex numbers \(z\) are parametrised by three angles, viz.,
\[
z_{11} = e^{i \phi_1} e^{-i \frac{\phi_2}{2}} \cos \frac{\theta_1}{2}, z_{12} = e^{i \phi_1} e^{i \frac{\phi_2}{2}} \sin \frac{\theta_1}{2}
\]
(25)
The \(z\)'s are grouped in the vector \(z = (z_{11}, z_{12})\).

The isospin vector \(I\) turns out to be a useful definition:
\[
I_1 = z_1^\dagger z_1 = (\cos \phi_1 \sin \theta_1, \sin \phi_1 \sin \theta_1, \cos \theta_1)
\]
(26)
The angle \(\theta\) can then be interpreted as the latitude on the isospin sphere, whereas the angle \(\phi\) is the longitude, cf. Figure 11. The north and south pole of the sphere correspond to a staggered flux phase, with \(A - B\) and \(B - A\) staggering respectively, while the equator corresponds to the \(d\)-wave superconductor. For half filling, the rotations on the isospin sphere correspond to pure gauge transformations, meaning that spinon flux phases and \(d\)-wave superconductors are gauge-equivalent.

The way the \(SU(2)\) mean field theory is set up, is as follows. The spinons and holons are considered to be separate systems. As long as one rotates the spinons and holons together, \(SU(2)\) gauge symmetry gives the same mean field properties. If one fixes a gauge for the spinons, and then starts to rotate the holons independently, the mean field results for the energy will be different. The strategy we choose is to fix the spion gauge at the dSC
mean field state, whereas the holons will be rotated by the group element \( g_i \). It was shown in Eq. (24) that \( g_i \) can be decomposed into “Euler angles” \( \alpha_i, \theta_i \), and \( \phi_i \). These can be encoded in the useful concept of isospin, as defined in [26]. We pictured this concept in the isospin sphere, cf. Fig. II. Only the angle \( \theta_i \) will turn out to be physical, whereas the other ones are gauge. For equator states, we have \( \theta = \frac{\pi}{2} \), corresponding to \(< b_1 > = < b_2 >= 0\), whereas for \( \theta = 0 \), \(< b_1 >= 0 \) and \(< b_2 >= 0 \). The latter means that the symmetry between empty sites and doubly occupied sites is broken.

The concept of isospin will turn out to be important for the last section, since it can encode for inhomogeneous states as \( \theta_i \) might vary with lattice site \( i \). But before turning to that topic, we need to cross some terrain.

### III. LESSONS FROM THE EMPTY LIMIT

In this section, we investigate the consequences of the peculiar form of the expression for the hole in the \( SU(2) \) formulation. We will demonstrate in the first subsection that the spinon pair involved will give rise to an \( s \) wave component in the spinon pairing parameter. Furthermore, we will show that the constraint equations lead to requirement of the bosons to have a hard core. This property will also take care of the mean field energy to be correct in the empty limit. In the last subsection it is demonstrated that the proposed mean field wave function even renders the single-electron propagator correctly.

Let us first discuss the hard-core nature of the holons. The exact wave function describing the empty limit is simple,

\[
|0\rangle = \prod_i \left( b_{1i}^\dagger + b_{2i}^\dagger f_{1i}^1 f_{1i}^\dagger \right) |\text{vac}\rangle. \tag{27}
\]

Deconfinement or spin-charge separation implies that the system loses its knowledge about the three particle correlation \( b_{1i}^\dagger f_{1i}^1 f_{1i}^\dagger \), and the best one can do is to look for a holon-spinon product wave function. The best choice is obviously

\[
|0\rangle_{MF} = \prod_i \frac{1}{2} \left( b_{1i}^\dagger + b_{2i}^\dagger \right) \left( 1 + f_{1i}^1 f_{1i}^\dagger \right) |\text{vac}\rangle. \tag{28}
\]

This wave function still has to satisfy the mean-field version of the constraint Eq. (28),

\[
\langle \psi_i^1 \tau^0 \psi_i + b_i^1 \tau^0 h_i \rangle = 0, \tag{29}
\]

where the brackets in this case stand for the expectation value relative to the state \( |0\rangle_{MF} \). This brings us to the main point: the constraints are only satisfied when the bosons have hard cores. Indeed, the mean field wave function Eq. (28) obeys

\[
\langle 0 | \, \psi_i^1 \tau^3 \psi_i \, |0\rangle_{MF} + \langle 0 | \, h_i^3 h_i \, |0\rangle_{MF} = 0 + 0 = 0. \tag{30}
\]

If we were to take soft-core bosons, the state \( (b_{1i}^\dagger)^2 + b_{2i}^\dagger |\text{vac}\rangle \) would be possible. It does not satisfy the constraints, however, since then

\[
\langle 0 | \, \psi_i^1 \tau^3 \psi_i \, |0\rangle_{MF} + \langle 0 | \, h_i^3 h_i \, |0\rangle_{MF} = 0 + 1 \neq 0. \tag{31}
\]

So, if we are to take the Hilbert space constraints seriously, we need to accept that the holons have an infinite hard core. This is consistent with the fact that the holons carry electric charge. Since the Coulomb repulsion is taken infinite to arrive at the \( t-J \) model in the first place, this means that there can be at most one \( b \)-boson per site.

The reason to stress this hard-core nature of the bosons, is that in the original formulation, the bosons were taken to be non-interacting. The empty limit exercise, being transparent in this regard, shows that this is inconsistent for appreciable dopings. This is also illustrated by the fact that the hard-core bosons give the correct energy in the empty limit. Indeed, let us first show that with the original projected electrons, the exact energy of the \( t-J \) Hamiltonian Eq. (11) is zero in this limit. The empty state is described in the projected electron formulation simply by \(|\text{vac}\rangle\), implying vanishing \( n_i \) on this state. Since the spin operator \( S_i^z \) is given by \( \epsilon_{\alpha\beta} \frac{1}{2} \gamma_i^\dagger \gamma_i c_{\alpha i} c_{\beta i} \), the energy of the Heisenberg part vanishes. Since there are no electrons around, the hopping part vanishes as well, and we conclude that the total energy vanishes.

Let us now demonstrate that the Ansatz Eq. (28) yields the same result. Firstly, the Heisenberg term vanishes.
The only component of spin that could contribute is the $\alpha$ = 3 component, since the others vanish when acting on $|1 + f^\dagger_{11}f^\dagger_{11}|\text{vac}\rangle$. However, since $S^3$ is the number of up spins minus the number of down spins, it vanishes as well. Furthermore, since the number operator $n_i$ in the slave boson representation reads $c^\dagger_{ia}c_{ia} = \frac{1}{2} [\hat{h}_i^\dagger\hat{h}_i^\dagger]|\psi_i\rangle$, it also gives zero contribution, because of the hard core condition. Similarly, the hoppings vanish for the same reason.

This would not be the case if the bosons were assumed to have no hard core, since for weakly interacting bosons there is no restriction on the hoppings. This is inconsistent with the $t$ – $J$ model, as hopping is only allowed between occupied and empty sites. In conclusion, the hard core condition is a sufficient condition for the empty state to have the correct energy in the empty limit.

So far, we have derived an exact expression for the hole creation operator in the SU(2) gauge theory, taking seriously all three constraints. We considered the empty limit first, since it is easy to construct the mean field theory in this case. Treating the constraints correctly, we arrived at the conclusion that the bosons should be treated as having a hard core. In the next section, we will show how our mean field Ansatz Eq. (28) generalises to mean field wave functions describing intermediate dopings.

A. Doping induces an s-wave order parameter

In the previous section, we showed that a correct description of the empty limit requires that the bosons should be treated as hard-core. The empty limit considerations lead us to that conclusion, turns out to be very useful to find out the structure of the mean field wave function at intermediate dopings. In fact, hard-core bosons are just like XY spins, and the straightforward generalisation of Eq. (28) becomes obvious,

$$|\Psi_0\rangle_{\text{holons}} = \prod_i \left( \alpha_i + \beta_i (u_i b^\dagger_{i1} + v_i b^\dagger_{i2}) \right) |\text{vac}\rangle,$$

where the complex numbers $\alpha$ and $\beta$ obey the normalisation condition $|\alpha|^2 + |\beta|^2 = 1$.

To already harvest some results from our considerations, let us consider the saddle point Lagrange multiplier equations

$$\frac{\partial}{\partial a_{il}} \langle H_{mf} \rangle = 0, \quad l = 1, 2, 3.$$  

(33)

These are precisely the mean field constraint equations Eq. (28):

$$\langle f^\dagger_{i1} f^\dagger_{i1} + f_{i1} f^\dagger_{i1} \rangle = \langle b^\dagger_{i2} b_{i2} + b^\dagger_{i1} b_{i1} \rangle.$$

(34)

$$\langle f^\dagger_{i1} f^\dagger_{i1} - f_{i1} f^\dagger_{i1} \rangle = -i \langle b^\dagger_{i1} b_{i2} - b^\dagger_{i2} b_{i1} \rangle.$$

(35)

$$\langle f^\dagger_{i1} f_{a3} - 1 \rangle = \langle b^\dagger_{i3} b_{i2} - b^\dagger_{i3} b_{i3} \rangle.$$

(36)

These constraint equations already convey an important message. The third equation tells us something about the deviation from half-filling, which was an important point already made by Lee, Wen and Nagaosa (2). As soon as the average fermion occupation number deviates from unity, i.e., deviates from half filling, there is a difference between $b_1$ bosons and $b_2$ bosons. In plain physics language: as soon as Fermi pockets form, the difference between empty sites and spin pair singlets becomes physical.

The first two equations acquire a novel interpretation. For non-zero dopings, the holon expectation values are non-zero as well. However, looking at the left-hand side of the equations, one needs to conclude that a superfluid order parameter appears with an s-wave structure. In other words, taking seriously all constraint equations, and having convinced oneself that doping must be described by a superposition of both empty and doubly occupied sites, one has to face an extra order parameter with a superconducting s-wave symmetry. Rephrased in physical language: within the framework of SU(2) theory, doping induces s-wave pairing.

One could argue that there are some left-over degrees of freedom, so that one could gauge away the s-wave component. This is not the case, however. Let us exploit the isospin representation, introduced in Section II, using the isospin angles $\varphi$ and $\theta$, cf. Fig. III we parametrise the holon wave function (32) by $u_i = \cos(\frac{\varphi_i}{2})$ and $v_i = \sin(\frac{\varphi_i}{2})$. Further, choose $\beta_i \rightarrow \beta_i e^{i\varphi_i}$ such that $\beta_i$ is real. This parametrisation is instructive, since $\theta_i = \frac{\pi}{2}$ makes the expectation values for $b_1$ with vacancies indistinguishable from $b_2$ with a spinon pair, reproducing the particle-hole symmetric empty state Eq. (28). Moreover, this corroborates the point that the equator on the SU(2)-isospin sphere (i.e., $\theta_i = \frac{\pi}{2}$) corresponds to the particle-hole symmetric d-wave superconductor. Calculating the expectation values explicitly, the equations Eq. (28) become

$$\langle f^\dagger_{i1} f^\dagger_{i1} + f_{i1} f^\dagger_{i1} \rangle = |\beta_0|^2 \sin(\theta_i) \cos(\varphi_i).$$

(37)

$$\langle f^\dagger_{i1} f^\dagger_{i1} - f_{i1} f^\dagger_{i1} \rangle = |\beta_0|^2 \sin(\theta_i) \sin(\varphi_i).$$

(38)

$$\langle f^\dagger_{i1} f_{a3} - 1 \rangle = |\beta_0|^2 \cos(\theta_i).$$

(39)

On the one hand, this illustrates once again that equator states are particle-hole symmetric, cf. Eq. (39). Secondly, and more importantly, we see that there is no way to gauge away the s-wave component. In other words, as soon as there is a superconducting order parameter ($\sin(\theta) \neq 0$), there is an s-wave component linearly increasing with doping $x$:

$$\Delta_s = \frac{1}{2} x \sin(\theta).$$

(40)

The only freedom is to choose its phase to be real by choosing $\varphi_i = 0$, implying zero $\beta_0^2$. This is a first result of our empty-limit exercise, which at first sight looks trivial. Conversely, the first equation tells us that we cannot
neglect the Lagrange multiplier $a_{01}^1$, which accounts for the $s$-wave admixture. This has been ignored in the original formulations of the mean field theory. This flaw leads to a disaster, as we will show in the next subsection.

**B. The Empty Limit in Mean-field Theory**

One could wonder if it is really wrong to leave out the first constraint. Probably one remains very closely to the "correct" mean field state when ignoring it? This is not the case: it leads to nonsensical results. The bright side is the ease by which the constraint $a_{01}^1$ is incorporated.

Let us fix the holon density $\langle h_i^1 h_i \rangle = 1$, and choose the Hubbard-Stratonovich fields to be homogeneous, $\Delta_{ij} = \Delta, \chi_{ij} = \chi$. Since the empty state makes no distinction between empty and doubly occupied sites, we have $\theta_i = \theta = \frac{1}{4}\pi$. Inserting these assumptions into Eq.(14), we obtain an energy density functional $E_{m\text{f}}$ for the empty limit.

Let us first ignore $a_{01}^1$. Then the mean field equations are

$$\frac{\partial E_{m\text{f}}}{\partial \chi} = 2\chi = \sum_k \frac{\chi(\cos k_x + \cos k_y)^2}{E_k},$$

$$\frac{\partial E_{m\text{f}}}{\partial \Delta} = 2\Delta = \sum_k \frac{\Delta(\cos k_x - \cos k_y - a_{01}^1)(\cos k_x - \cos k_y)}{E_k},$$

$$a_{01}^1 = 0.$$  \hspace{1cm} (41)

where the dispersion $E_k$ is given by

$$E_k = \sqrt{\left(\chi_k - a_{01}^1\right)^2 + \left(\Delta_k - a_{01}^1\right)^2},$$

$$\chi_k = -\frac{3J}{4}\left(\cos k_x + \cos k_y\right)\chi,$$

$$\Delta_k = -\frac{3J}{4}\left(\cos k_x - \cos k_y\right)\Delta.$$  \hspace{1cm} (42)

In the empty limit, the holons cannot move, so there are no mean field equations and dispersions governing those. The above mean field equations can be solved numerically to yield the unphysical result $\chi = \Delta = \frac{\sqrt{2}}{2}$, identical to the result for half filling. But this is clearly nonsense: the empty limit is neither a spin liquid nor a superconductor. Also, since $\Delta$ and $\chi$ are non-zero, the total energy will be non-zero, in flagrant contrast with the correct result being zero, as pointed out earlier.

Taking $a_{01}^1$ into account, however, the above mean field equations are extended with the saddle point equation for $a_{01}^1$,

$$1 = \sum_k \frac{\Delta(\cos k_x - \cos k_y) - a_{01}^1}{E_k},$$  \hspace{1cm} (43)

where the number 1 is the boson density. Solving the new system of equations numerically, we obtain the correct result $\chi = \Delta = 0$ and $a_{01}^1 = \frac{1}{2}$. Therefore, the Lagrange multiplier is of central importance, and the mean fields vanish, as they should. Substituting this solution in the Hamiltonian Eq.(13), we recover the correct energy for the empty limit. In other words, things go dramatically wrong if $a_{01}^1$ is ignored. In Section IV we will show that our mean field theory is performing well as an energy density functional at intermediate dopings. To calculate dynamic properties, one has to be careful in choosing the correct mean field approach.

**C. Dynamical Properties of the Empty Limit**

It is interesting to consider the dynamical properties following from the slave boson theory in the empty limit. It turns out that although this theory is a good energy functional, it is less trustworthy with regard to dynamical properties revealed through the propagators. This is of course due to the mean field treatment ignoring fluctuations of the gauge fields. Indeed, the Lagrange multipliers $a_{01}^1$ should be given dynamics, causing fluctuations confinement of the spinons and holons to electrons. Since we ignored the fluctuations, we can not expect the mean field theory to describe the physical electron of the empty limit.

The starting point for the study of electron dynamics is the single electron propagator

$$G(x,y;t-t') = \langle \langle c_{x\uparrow}(t) c_{y\uparrow}^+(t') \rangle \rangle$$  \hspace{1cm} (44)

Here the $c_{i\sigma}$ again describe projected electron operators. Since in the empty limit there are by definition no electrons in the vacuum,

$$G(x,y;t-t') = \sum_{kk'} e^{ikx-iky} \langle c_{k\uparrow}^1 e^{-i\hat{H}(t-t')/\hbar} c_{k'\uparrow}^1 \rangle \Theta(t-t')$$

$$\times \Theta(t-t') e^{iE_0(t-t')/\hbar}.$$  \hspace{1cm} (45)

Let us first show that for the exact expression (27) describing the empty limit of the $t-J$ model, one obtains a free particle dispersion. We need to know the time evolution operator $e^{-i\hat{H}(t-t')/\hbar}$. The Hamiltonian operator has no Heisenberg part for projected electrons, and it also vanishes on the state $c_{x\uparrow}^1 |0\rangle$, where $|0\rangle$ is the wave function Eq.(27). So we only need to calculate the effect of $H_t = -t \sum_{ij} \psi_j^+ h_i h_j^+ \psi_j$ on

$$\langle c_{k\uparrow}^1 H_t c_{k1}^+ \rangle = -2t \delta_{kk'}(\cos k_x + \cos k_y) \equiv \varepsilon_k \delta_{kk'}.$$  \hspace{1cm} (46)

In Fourier space, the result is

$$\langle c_{k\uparrow}^1 H_t c_{k1}^+ \rangle = -2t \delta_{kk'}(\cos k_x + \cos k_y) \equiv \varepsilon_k \delta_{kk'}.$$  \hspace{1cm} (47)
Including the chemical potential and using a contour integral expression for $\Theta(t-t')$, we conclude that the propagator is

$$G_{exact}(k, \omega) = \frac{1}{\hbar \omega - (\varepsilon_k - \mu) + i\eta},$$

(50)

the correct result for the propagator of a free particle. This means that the wave function Eq.\,(27) encodes the right physics, as expected.

What performance can be expected from the mean field theory when asked dynamical questions? Let us first consider the case for the mean field Hamiltonian Eq. (13). Without $a_0^\dagger$, one obtains the expected errors, namely a $d$-wave dispersion. Repairing this with a nonzero $a_0^\dagger$ leads, however, to just partially good news. We showed that the $d$-wave dispersion vanishes, which is physical. The bad news, however, is that both $\chi$ and $\Delta$ are zero. This absence of kinematics would lead to a dispersionless spinon spectrum. This is not what one would expect, since shooting electrons into the void should behave as a free electron cosine dispersion.

This motivates the second approach: let us apply only mean-field theory at the wavefunction level, without introducing the Hubbard-Stratonovich fields Eq.\,(10) and Eq.\,(11). This means that the Hamiltonian then reads

$$H_{exact} = -\mu \sum_i h^\dagger_i h_i - \sum_i a_0^\dagger \left( \frac{1}{2} \psi^\dagger_{\alpha i} \tau^\dagger \psi_{\alpha i} + h^\dagger_i \tau^\dagger h_i \right) + \sum_{<ij>} \frac{3J}{8} (S_i \cdot S_j) - \sum_{<ij>} t \left( \psi^\dagger_i h_{ij} \psi_j + h.c. \right).$$

(51)

In the empty limit, we just have one contribution to the propagator

$$G_{mf}(x, y; t - t') = \sum_{kk'} e^{ik'x - iky} \langle c_{k'\uparrow}^\dagger e^{-iH(t-t')/\hbar} c_{k\downarrow} \rangle \times \Theta(t-t').$$

(52)

The expectation values are taken with respect to the empty-limit mean field state Eq.\,(28), denoted by $|0\rangle_{MF}$. It is convenient to first calculate how the electron operator acts on the empty limit mean field state,

$$c_{x\uparrow}^\dagger |0\rangle_{MF} = \frac{1}{\sqrt{2}} (b_{1x} f_{x\uparrow}^\dagger + b_{1x} f_{x\downarrow})$$

$$\times \prod_i \frac{1}{2} (b_{i\uparrow} + b_{i\downarrow}) (1 + f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger) |\text{vac}\rangle = \frac{1}{\sqrt{2}} f_{x\uparrow}^\dagger P_x |\text{vac}\rangle,$$

(53)

with the definition $P_x = \prod_x \frac{1}{2} (b_{0x}^\dagger + b_{0x}^\uparrow) (1 + f_{0x}^\dagger f_{0x}^\dagger)$.

First we demonstrate that the state $c_{x\uparrow}^\dagger |0\rangle_{MF}$ is a physical state, i.e., it satisfies the constraint Eq.\,(12). It does, since $b_{0x} P_x |\text{vac}\rangle = 0$ makes the expectation value $\langle h^\dagger x \tau^\dagger h_x \rangle$ zero. Furthermore, the fermionic expectation values vanish as well. As an example,

$$\langle 0 | c_{y\uparrow}^\dagger \psi_{x\uparrow}^\dagger \psi_{x\uparrow} \psi_{x\uparrow} \psi_{x\uparrow} | 0 \rangle_{MF} = \frac{1}{2} \langle 0 | P_y^\dagger f_y \psi_{x\uparrow}^\dagger f_{x\uparrow} \psi_{x\uparrow} \psi_{x\uparrow} | 0 \rangle_{MF} = \frac{1}{2}$$

$$= \frac{1}{2} \langle 0 | P_y^\dagger f_y \psi_{x\uparrow}^\dagger f_{x\uparrow} \psi_{x\uparrow} \psi_{x\uparrow} | 0 \rangle_{MF} = 0,$$

(54)

both for $x = y$ and $x \neq y$. The other $\ell$'s are checked similarly. This implies that the constraint terms in the Hamiltonian Eq.\,(11) vanish.

Then we demonstrate that the Heisenberg term also vanishes in $c_{x\uparrow}^\dagger |0\rangle_{MF}$. This can be seen easily since $S_i \cdot S_j f_{j\uparrow}^\dagger P_j |\text{vac}\rangle = S_j f_{j\uparrow}^\dagger S_i P_j |\text{vac}\rangle = 0$, by the same reason why the Heisenberg term of the mean field energy on the empty state vanishes.

Only the hopping terms are non-trivial. This is intuitively clear, since shooting an electron in the empty sample, removes one holon, allowing the rest to move. This is corroborated by calculating the matrix elements of the exact hopping Hamiltonian $H_t = -t \sum_{<ij>} \psi_{i\uparrow}^\dagger h_{ij} \psi_{j\uparrow}$:

$$\langle 0 | c_{y\uparrow}^\dagger H_t c_{x\uparrow}^\dagger | 0 \rangle_{MF}$$

$$= \frac{1}{2} \sum_{<ij>} \langle \text{vac} | P_y^\dagger (b_{1y} + b_{2y} f_{y\uparrow} f_{y\downarrow}) (b_{1x} + b_{2x} f_{x\uparrow} f_{x\downarrow}) P_x |\text{vac}\rangle = \frac{1}{2}$$

$$= \frac{1}{2} \sum_{<ij>} \langle \text{vac} | (1 + f_{x\uparrow} f_{x\downarrow}) (b_{1y} + b_{2y} f_{y\uparrow} f_{y\downarrow}) |\text{vac}\rangle$$

$$= \frac{1}{2} \sum_{<ij>} \delta_{ix} \delta_{ij},$$

(55)

meaning that the electron can only hop to a nearest neighbour site if that site is empty. The Fourier transform then reads

$$\langle 0 | c_{k\uparrow}^\dagger H_t c_{k\downarrow}^\dagger | 0 \rangle_{MF} = \frac{1}{2} \delta_{k,-k}(\cos k_x + \cos k_y) = \varepsilon_k \delta_{k,-k},$$

(56)

the free particle dispersion. This leads to the same free particle propagator as in the exact case,

$$G_{mf}(k, \omega) = \frac{1}{\hbar \omega - (\varepsilon_k - \mu) + i\eta}.$$  

(57)

In other words, when one treats the slave boson Hamiltonian exactly, the mean field wave function for the empty limit gives the correct single-electron propagator.

**IV. THE PHASE SEPARATED $d + s$-WAVE SUPERCONDUCTOR**

In the previous section, we have discussed how one should describe doping within the context of $SU(2)$ gauge theory. By studying this carefully, we convinced ourselves of two important lessons. The first one is that a hole in the $t-J$ model is described in the $SU(2)$ theory by a superposition of a vacancy and a spin pair singlet state. This implied that doping induces $s$-wave pairing.
The second message is that the holons describing doping should be hard core bosons, instead of gaseous, non-interacting particles employed by Wen and Lee. This hard-core is necessary condition in order to account for the fact that there can be at most one charge per site, as has been clear from very the beginning.

Our results are summarised in the mean-field phase diagram, reflecting the phase separated \( d + s \)-wave superconductor. Another ramification we make quantitative. The \( s \)-wave admixture in the superconducting gap is shown to shift the gap nodes along the Fermi surface. We predict how this node shift behaves as a function of doping. Indeed, a diagram, reflecting the phase separated stripes. Being aware of this complication, let us nevertheless study homogeneous states. Still, this exercise turns out to be instructive, in this regard. The reason is that we treat the Hamiltonian Eq. \((114)\) in the grand canonical ensemble, instead of the canonical ensemble. The original formulation of the SU(2) mean field theory \(8,9\) rested on the canonical ensemble as well. To account for condensation of the holons at finite doping, the temperature was taken to be finite, to find out that the particle number constraint leads to Bose-Einstein condensation of the holons, by treating \( \mu \) simply as a Lagrange multiplier. We prefer a different approach, since considering first finite temperature is a detour given in by the unphysical assumption that the holons form a non-interacting gas. On the other hand, hard-core bosons are not only more physical, but also easy to treat at zero temperature. In Section \(11\) we made the point that the bosons are interacting, making them superfluid at zero temperature. The last motive is the possibility of phase separation, i.e., the possibility of coexistence of phases with different densities at the same chemical potential in the same volume, giving rise to the need of performing the Maxwell construction. To anticipate this, it is necessary to take the chemical potential for the holons as control parameter, instead as the Lagrange multiplier enforcing a fixed density.

Let us substitute the mean field wave function Eq. \((58)\) in the slave Hamiltonian Eq. \((114)\), we obtain an expression for the mean field energy per site \( \frac{1}{N} \langle H_{MF} \rangle = e_{MF} \). \(N\) is the number of lattice sites.

\[
e_{MF} = -\frac{1}{N} \sum_k E_k + \frac{3}{4N} J(|\chi|^2 + |\Delta|^2)
- 2t\chi |\alpha|^2|\beta|^2 - (\mu + a_0^0 \sin \theta + a_0^0 \cos \theta)|\beta|^2.
\]

The homogeneity of the Ansatz is expressed in the fact that the lattice site subscript \( i \) is dropped. It is important to observe that the isospin latitude angle appears in the mean-field energy, expressing the fact that for nonzero doping, SU(2) gauge symmetry is broken. Hence \( \theta \) is not gauge, but has acquired physical meaning. The kinetic part of the energy is gauge invariant, leading to the fact that only the hoppings amplitude shows up in the holon hoppings. From this density functional, we derive the saddle point equations for the dynamical variables \( \chi, \Delta, a_0^0, a_0^0 \) and the hole density \( |\beta|^2 = \rho(\chi) = 1 - |\alpha|^2 \). To simplify matters a bit, we take the isospin angle \( \theta \) as an external parameter, controlling the density of \( b_2 \) relative to \( b_1 \).

The saddle point equations in the grand canonical ensemble are easily derived, with the homogeneous forms of Eq. \((57)\) and Eq. \((59)\),

\[
2\chi = \chi \sum_k \frac{\chi_k (\chi_k - a_0^0)}{E_k} + 2 \left( \frac{4t}{3J} \frac{\partial}{\partial \chi} \rho(\chi) (1 - \rho(\chi)) \right)
\]

\[
2\Delta = \Delta \sum_k \frac{\Delta_k (\Delta_k - a_0^0)}{E_k}
\]

\[
\rho(\chi) \sin(\theta) = \sum_k \frac{(\Delta_k - a_0^0)}{E_k}
\]

\[
\rho(\chi) \cos(\theta) = \sum_k \frac{(\chi_k - a_0^0)}{E_k}
\]

\[
0 = \rho(\chi) \left( \rho(\chi) - \frac{1}{2} \left( 1 + \frac{\mu + a_0^0 \sin \theta + a_0^0 \cos \theta}{2t\chi} \right) \right).
\]
As already discussed after Eq. (67), these equations give rise to an important law which provides a linear relationship between the $s$-wave spinon pairing $\Delta_s \equiv \langle f_i^\dagger f_{i'}^\dagger \rangle$ and the doping $x = \rho(\chi)$,

$$\Delta_s = \frac{1}{2} x \sin(\theta),$$

as a direct ramification of the full constraint structure.

In order to find the solutions to the saddle point equations Eq. (60), the energy Eq. (60) is minimised numerically using the simulated annealing method\textsuperscript{37,38}.

We point out that the fifth equation admits both zero and non-zero solutions for the density $\rho$. As a function of $\mu$, the mean field energy will tell which one is more favourable. In Section IV B, we will show that the system chooses between these two by a first order phase transition, and not a second order one! This means that the mean field theory\textsuperscript{39} implies a phase separation regime, for the usual Maxwell construction reasons, when transforming to the canonical ensemble.

**B. The $SU(2)$ mean field phase diagram**

We have now arrived at the point where we can collect the results. Our first step was to prove that one needs all $SU(2)$ constraints to project onto the $t - J$ model Hilbert space, while this constraint structure is also required for the mean field description of the $SU(2)$ gauge theory. This will bring us to the first result: that the superconducting order parameter needs to have an $s$-wave component! Then we spent effort in proving that the holons need to be hard-core in order to respect the full set of $SU(2)$ constraints. We now show that the superfluid hard-core holon condensate displays phase separation behaviour, as expected for hard-core interacting systems. We thereby achieve an intrinsic connection between slave theories on the one hand, and the observation of inhomogeneous states for low doping. As a function of increasing $J/t$ the width of this phase separation regime is increasing (see Fig. 2) and we find that for $J/t \approx 4$ the phase separation is complete. This is consistent with exact diagonalisation studies on the $t$-$J$ model indicating a complete phase separation for $J/t \geq 3.5\textsuperscript{15,39}$. This is quite remarkable and it reveals that the gauge mean field theory has to be a remarkably accurate quantitative theory of the density functional kind: it is a good description of the empty limit and the Mott insulator, and gives a fair prediction of phase separation tendencies. We stress that as a rule less severe demands on physical reality are put on density functional theory, instead of full dynamical theories.

We stress here that this phase separation behaviour is eventually coming from the hard-core nature of the holons: also the ”wrong” mean field states (SFP and pure dSC with pockets) exhibit first order behaviour. We conclude that, due to the Hilbert space restrictions on the $SU(2)$ description of the holons, the theory insists on inhomogeneous states for low doping. As a function of $J/t$ the width of this phase separation regime is increasing (see Fig. 2) and we find that for $J/t \approx 4$ the phase separation is complete. This is consistent with exact diagonalisation studies on the $t$-$J$ model indicating a complete phase separation for $J/t \geq 3.5\textsuperscript{15,39}$. This is quite remarkable and it reveals that the gauge mean field theory has to be a remarkably accurate quantitative theory of the density functional kind: it is a good description of the empty limit and the Mott insulator, and gives a fair prediction of phase separation tendencies. We stress that as a rule less severe demands on physical reality are put on density functional theory, instead of full dynamical theories.

The significance of this finding is that for this most sophisticated version of spin-charge separation theories, phase separation is natural feature, as it is in the empirical reality. It is well understood that these macroscopic phase separated states are an artefact of the oversimplified $t - J$ model. By taking the long-range Coulomb interaction into account this will turn immediately into the microscopic inhomogeneity\textsuperscript{13,15,49} of the

![FIG. 2: Chemical potential shift as a function of doping, showing the phase separation behaviour of the reformulated mean field theory. Indeed, the chemical potential starts to shift for appreciable dopings only. The blue line (colours online) are the numerical results for $J/t = 0.1$, and agrees very well with the experimental results from Fujimori\textsuperscript{13} (dotted line). The red line are the results for $J/t = 0.3$. The critical doping changes, but not the compressibility. The inset shows that ignoring $a_0^\dagger$, i.e., ignoring the $s$-wave component, gives a false vacuum. Indeed, there is a positive relative energy difference between the pure dSC and our mean field theory, growing with doping (lower line).](image)
kind that are seen in STM-experiments. To see how well this slave theory handles the ‘big numbers’ in this regard, we show in Fig. 1 the electronic incompressibility \( 1/\kappa = \frac{\partial^2 E_{\text{MF}}}{\partial \rho^2} = \frac{\partial^2}{\partial \rho^2} \) according to the SU(2) theory, to find that it compares remarkably well with the experimental results due to Fujimori and coworkers. Firstly, it is seen that independent of the ratio \( J/t \), the compressibility is right on spot of the experiments: the slope of \( \mu \) vs. holon density is the same as the measured slope. The doping at which phase separation occurs, namely 13 %, is correct only for the value \( J/t = 0.1 \), which is too small. Indeed, from ARPES measurements a ratio of \( J/t = 0.3 \) is more realistic, but for those samples phase separation takes place at dopings of about 17 %, and not 21 %, as found in the SU(2) mean field theory for \( J/t = 0.3 \).

Let us now focus on the nature of the superconducting order parameter found elevated doping levels. As expected, the s-wave component becomes increasingly important, cf. Eq. (50). To further emphasize this, we compare in the inset of Fig. 1 the energy of a state where we have fixed the Lagrange multiplier \( a_0^1 = 0 \) such that the s-wave component vanishes, with the best \( d + s \) mean-field state, finding that the former is indeed a false vacuum. To mimic the average behavior of the superconducting order parameter also in the micro-phase separated states at low dopings, we calculate matters now in the false (uniform) vacuum of the canonical ensemble, fixing the average density, simplifying the mean field equations Eq. (54). Indeed, \( \rho(\chi) \) becomes now a fixed \( \rho \). Furthermore, since the state \( \theta = \frac{\pi}{4} \) is favoured, we take the mean field Ansatz \( U_{ij} \) to be the SC one, as stated before, and consequently we have \( a_0^3 = 0 \). This enables us to map out the phase diagram as a function of doping and the ratio \( J/t \), leading to three phases. The first, for low doping, is the phase-separated, underdoped \( d + s \)-wave superconductor. It is a mixture of charged, superconducting islands in an insulating sea without charges, where the full SU(2) symmetry is restored. This reminds the reader of the STM-pictures from S.C. Davis’ group. For intermediate dopings, the homogeneous, overdoped \( d + s \)-wave superconductor is found, whereas for high dopings, the \( d + s \) gap vanishes, leaving behind a pure \( s \)-wave superconductor. Hence, although \( d \)-wave superconductivity leads to an \( s \)-wave admixture, the reverse is not true.

We find that the regime where phase separation is important, the \( s \)-wave component is not negligible. This is consistent with Raman measurements, where the superconducting gap was found to have both \( d \)- and \( s \)-wave components. Although screening effects in Raman scattering make it difficult to compare our results directly to theirs, their results indicate that the ratio \( r = \Delta_s/\Delta_d \) grows with doping, as it does in our approach. Looking to Figure 3, we find in the phase separated overdoped regime \( s \)-wave admixtures of about \( r = 10 - 20 \% \), consistent with c-axis tunneling experiments.

We predict that at a doping level that appears to be higher than can be achieved in cuprate crystals a phase...
transition occurs to a pure s-wave superconductor. As we already alluded to, the gauge fluctuations should become more severe as well, for increasing doping and at some doping level a transition should occur to a confining "electron like" system.

As we learned from the empty limit, it still make more sense than the result obtained by disregarding the first constraint equation Eq. (37), since that would lead to the unphysical result \( \chi = \Delta = \frac{1}{V} \), giving the wrong vacuum energy, as we discussed in Section III. In other words, our mean field theory is a remarkably good density functional theory, but inevitably the theory fails completely in dynamic regards. In the confined phase, at sufficiently high dopings, we need an approach which is qualitatively different from slave theories, let alone that one can get away from the mean field version. On the other hand, in the superconducting doping regime, we find some promising experimental support for our results with regard to the d+s structure of the order parameter, meaning that confinement physics might not be overwhelmingly important in the low-doping part of the phase diagram.

Having said this, the experimental support for an s-wave admixture makes it possible to come up with a falsifiable prediction for photo-emission experiments. The s-wave component induces a shift in the nodes, as can be inferred from the spinon dispersion \( E_k \), Eq. (17): the hopping vanishes along the line \( k_y = \pi - k_x \), so that the node of the order parameter can be readily calculated to be \( k_y - \frac{1}{4}\pi = \arccos(a_0^2/(3J/2\delta)) \), which shows a doping-dependent behaviour as well, cf. the blue line in Figure 3. The node shifts might be able to explain the U-shaped gap as measured in Bi2212, since the twinning of samples mixes regions of node shifts +\( \delta \) with -\( \delta \), smearing out the V-shape of the gap to a U-shape.

### C. Single-electron dynamics

It is also possible to interrogate the single-electron dynamics of the superconducting state. Wen, Lee, Nagaosa and Ng have addressed this issue for non-interacting holons\( \delta \). Since we showed that one cannot ignore the hard-core nature of the holons for appreciable dopings, it is interesting to investigate what the electron correlation function looks like. We will demonstrate that it consists of two parts, ubiquitous in hard-core interacting Bose systems\( \delta \): one is a coherent condensate piece, and the second is an incoherent piece displaying sound modes for long wavelengths. This novel result is entirely due to the hard-core nature of the bosons, and might lead to falsifiable experimental predictions.

The calculation can be a bit simplified by the fact that in the superconducting state \( \theta = \frac{1}{2}\pi \), hence we write \( b_1 = b_2 = b \). Then the electron propagator

\[
G(k, t - t') = \langle \langle c_k(t)c_k^\dagger(t') \rangle \rangle
\]

is the convolution of bosonic operators \( b_p \) and \( f_{k+p} \), which can be seen by Fourier transforming the expression for the electron \( c_{q\uparrow} = b_{q\uparrow}^\dagger f_{q\downarrow} + i b_{q\downarrow} f_{q\uparrow}^\dagger \). The time resolved propagator \( G(k, \omega) \) can be calculated by using the spinon coherence factors \( u_{k+p} \) and \( v_{k+p} \) from the Bogoliubov diagonalisation of the spinons

\[
\begin{align*}
    f_{q\uparrow} &= u_q\gamma_0 + v_q\gamma_1^\dagger \\
    f_{q\downarrow}^\dagger &= -v_q\gamma_0 + u_q\gamma_1
\end{align*}
\]

Exploiting the Fourier transformation of the textbook result\( \delta \) for the boson propagator, the frequency resolved propagator then reads for finite repulsion \( U \)

\[
G(k, \omega) = \sum_p \int \frac{d\Omega}{2\pi i} \left\{ \frac{-|u_{k+p} - v_{k+p}|}{(\hbar\omega - \hbar\Omega + \varepsilon_{k+p})} + i\eta \left[ x_0\delta(p)\delta(\Omega) - \frac{\hbar(\Omega + \Omega_p)}{\hbar^2(\Omega_p - \Omega)^2 - (2Ux_0)^2} \right] \right. \\
&\quad + \left. \frac{|u_{k+p} + v_{k+p}|}{(\hbar\omega - \hbar\Omega + \varepsilon_{k+p}) - i\eta} \right\} \left[ x_0\delta(p)\delta(\Omega) + \frac{\hbar(\Omega + \Omega_p)}{\hbar^2(\Omega_p + \Omega)^2 - (2Ux_0)^2} \right] \right. \\
&\quad + \left. \frac{\hbar^2\Omega}{\hbar^2(\Omega_p - \Omega)^2 - (2Ux_0)^2} \right\}.
\]

Here, the fermion and boson dispersions are denoted by \( \varepsilon_k \) and \( \hbar\Omega_p \), respectively. Although the expression for
the propagator Eq. (64) seems lengthy at first, it conveys a couple of important messages. The most obvious one is the fact that the propagator is a convolution of bosons and fermions. The second one is the separation between the condensate piece, proportional to $x_0$, and an incoherent piece. The condensate piece leads to poles at the fermion dispersions, $h\omega = \varepsilon_{k+\mu}^i$. The incoherent piece is even more interesting. Since for the bosons $h\Omega_p = 2t\chi(\cos k_x + \cos k_y)$, we have for the long wavelength limit and for $\mu \approx 2t$ (the requirement for a condensate to exist) that the holon poles are located at

$$h\Omega \approx 2t\chi \sqrt{2U x_0 |k|} \ \text{ finite } U. \quad (65)$$

The holon velocity of sound can be written in a form for hard-core bosons as well, since for finite $U$, $x = \frac{1}{2U} (2t\chi + \mu)$, whereas for hard core bosons $2t\chi + \mu = 2x_0$. Hence the result Eq. (65) can be generalised to infinite repulsion $U$,

$$h\Omega = 2(2t)^2 \sqrt{x_0 |k|} \ \text{ infinite } U. \quad (66)$$

This means that for the incoherent piece of the propagator Eq. (64), the poles are located at

$$h\omega = \varepsilon_{k+\mu}^i - v |k|, \ \ k \to 0. \quad (67)$$

with the velocity of sound $v = 2(2t)^2 \sqrt{x_0}$.

In summary, we have argued that in order to achieve consistency in the $SU(2)$ slave boson theory, one has to implement hard-core bosons instead of gaseous Bogoliubov bosons to describe the charge sector. As a result, one obtains phase separation at lower dopings consistent with the experimental observations. Also the compressibility matches very well. Furthermore, by inspecting the empty limit, we showed that an $s$-wave component in the superconducting order parameter is implied when $d$-wave superconductivity occurs, at least for dopings where homogeneous states exist, a ramification of the constraint structure. This finds its origin eventually in the particle-hole symmetry central to the gauge structure of the $SU(2)$ theory: to describe physical spin singlets, “no fermions” are indistinguishable from an “$s$-wave spinon pair”. This is reflected in the constraint equations, required to reduce the $SU(2)$ Hilbert space to the Hilbert space of the $t-J$ model. The constraint equations tell us that as soon as $d$-wave superconductivity emerges, one necessarily has an $s$-wave component. This $s$-wave admixture is in accord with Raman and $c$-axis tunneling experiments. We also predict a node shift in the gap function, that might be measurable by photoemission.

V. ISOSPIN SPIRAL STATES IN CUPRATES

Having established the phase separation tendencies, new perspectives are opened as to what the role of stripes in the superconducting cuprates is. The understanding is that phase separation is a necessary condition for stripes to exist. On the other hand, phase separation has never been seen in the high-$T_c$’s. In fact, there are other properties at work. The Mott insulator is an antiferromagnet, which makes it advantageous for holes to order in stripes instead of phase separated islands. In fact, stripes should be regarded as antiphase boundaries in the antiferromagnet.

In the past decades, many approaches to understand the Hubbard model in some slave boson representation are made. One is the large-$S$ expansion, taking the limit of the spin value $S \to \infty$. The other is introducing more than two flavours of spin, such that an $SU(N)$ model is obtained. The large-$N$ limit leads to dimerised states, whereas the vacuum of the large-$S$ limit is the antiferromagnet. The question arises if the group $SU(2)$ is able to describe the “anti-phase boundaryness” of the antiferromagnet, the more so since the antiferromagnet and the dimerised state are incompressible, whereas the flux phases and the dSC spin liquids of the $SU(2)$ theory are compressible.

We propose a way in which the $SU(2)$ mean field theory can describe anti-phase boundaries, within the spin liquid states descending from the Mott insulator. The first observation is that for zero doping, the dSC or SFP state is just a gauge fix within the same projective symmetry group. Let us now consider a gauge in which the spinon mean field $U_{ij}$ Eq. (13) rotates over the whole isospin sphere,

$$U_{ij} = \exp(i(-1)^i \theta_i \tau^1) \left( \begin{array}{cc} \Delta & \chi \\ -\chi & \Delta \end{array} \right) \exp(-i(-1)^i \theta_i \tau^1)$$

by a harmonically varying isospin angle

$$\theta_i = Q \cdot i = q_i x, \ \ \text{ordering vector } Q \ \text{in } x \ \text{direction. \quad (69)}$$

In this way, the SFP state is smoothly connected to a dSC state. Observe that this state is in the same PSG for zero doping. Then the idea is that for underdoped samples this spiral state might be lower in energy than the phase separated state for the homogeneous $d+s$-wave superconductor. A cartoon representation is given in the figure.

The peculiar feature of the isospin spiral is that in the $SU(2)$ gauge theory the charge-density wave is made out of a superconductor, which is not the case in the large-$S$ limit. The antiferromagnetic domains are now replaced by a spin liquid, carrying nodal fermions, a feature absent in the antiferromagnet. As the nodal fermions exist in both the dSC and SF phases, a very promising perspective is opened up, supported by experiments.

The first support comes from the results from Fujimori and coworkers and Z.X. Shen and collaborators for LaSCO. The chemical potential shift measurements of Fujimori in underdoped LaSCO are compatible with the existence of charge order, with Shen finding similar results. Furthermore, in the Nd-doped cuprates,
clear features of static stripes are measured already in the nineties. The combination of these results seem to indicate the coexistence of striped charge order with nodal fermions. This idea is backed by recent results from the group of J.C. Davis, reporting that charge order and nodal fermions can coexist.

The SU(2) gauge theory is able to capture 'Mottness', d-wave superconductivity and the protection of nodal fermions. The framework of the isospin spiral state in the SU(2) mean field theory forms an excellent explanation to explain the mystery why nodal fermions should exist in a strongly correlated background. This is a promising motivation to study the stability of the isospin spiral mean field states in underdoped cuprates.

As a first attempt, we adapted our program such that it can incorporate inhomogeneous constraints, within the harmonic approximation. We used a 2×8 unit cell, as suggested in Figure 6. Via simulated annealing, a self-consistent solution can be found for chemical potentials µ admitting inhomogeneous boson densities. In Figure 7, the mean field energy as a function of average doping is plotted, together with the energy of the homogeneous solution.

It can be seen that the homogeneous states are better in energy in the homogeneous regime (x > 20% for J/t = 0.3). One expects that in the phase separation regime, the isospin spiral state wins. Unfortunately, the spiral state is energetically a little bit less favorable the homogeneous state, but this is an artefact of the unrealistic t−J-model. Any model which is closer to the experimental reality, admitting stripes in the underdoped regime, are expected to favor the spiral states. This hope is corroborated by the fact that the energy differences with the homogeneous state are small, i.e., a couple of percent. The direction of future research is clear: do models supporting stripes, also support isospin spiral states in the SU(2) slave boson formulation? This question is of high importance in the underdoped regime.

In that regime, it is interesting to see whether there can be made a “Yamada-plot” of the isospin speed Q as a function of doping x, since Q induces period 2Q-stripes.

In addition, we can shed some light on the issue of the coexistence of nodal fermions with stripes. We determined numerically the dispersion relations for the spinons for the Q = π/8 spiral, on a 8×2 unit cell. We only took the spinon part of the propagator into account. The result is shown in Fig. 8.

The surprising result is that there is no appreciable Umklapp scattering in the spinon sector, at this resolution at least. It is interesting to calculate the full electron spectral density, taking both the inhomogeneities in the boson condensate and the incoherent phonon part into account. We expect that the Umklapp might vanish altogether.

The Figure 8 might not be decisive, but very promising as to the idea that nodal fermions and stripes are not as mutually exclusive as thought for a long time in the high-Tc community. Further effort should be put in more precisely mapping out the nodal dispersion, especially in the underdoped regime.

In summary, we discussed how the constraint structure of the mean field SU(2) gauge theory of the doped Mott insulator forces the holons to have a hard core. This was demonstrated by considering the empty limit.
The momentum resolution is $\Delta k/a = 1/128$. The chemical potential was chosen such that the average doping was 26%, with variations (stripes) in hole density of 2%. The dispersion potential was chosen such that the average doping was 26%, with variations (stripes) in hole density of 2%. The dispersion across the spinon Fermi surface at $(\frac{1}{2}\pi, \frac{1}{2}\pi)$. It is seen that in contrast to usual belief, there is no appreciable Umklapp scattering. This result supports the idea that by the isospin spiral state, the nodal fermions coexist with stripes.

The empty limit was shown to produce the correct mean field energy, using the hard-core condition, and the correct single-electron propagator. As a surprise, we showed that an $s$-wave pairing in the spinon sector is inevitable, and grows linearly with doping. Then the mean field behaviour for intermediate dopings was shown to capture phase separation tendencies in the underdoped regime, being quantitatively in accord with both numerical results and experiments. The single-particle propagator was shown to display phonon modes.

We put forward indications that the $SU(2)$ gauge theory is able to capture both 'Mottness' and $d$-wave superconductivity in a unifying picture, introducing the concept of the isospin spiral. This idea might offer the possibility of the protection of nodal fermions, as the calculated spinon sector of the single electron spectral function seems to indicate. The framework of the isospin spiral state in $SU(2)$ mean field theory forms an excellent explanation to explain the mystery why nodal fermions should exist in a strongly correlated background. This is a promising motivation to study the stability of the isospin spiral mean field states in underdoped cuprates further, together with making predictions for ARPES measurements.

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