Planar and Stripe Orders of Doped Mott Insulators In Dual Spin Models

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We focus on very general, very large U, doped Mott Insulators with arbitrary hopping and interactions. We provide simple testimony to the competition between magnetic and superconducting orders in these systems. By mapping hard core bosons, spinless, and spinful fermions onto XXZ models, we aim to make very simple precise statements. We try to address optimal and expected filling fractions of holes within the plane and on stripes in a variety of hole and hole pair geometries. We examine the role of attractions/repulsion amongst hole pairs and single holes, and provide trivial expected numerical values for filling fractions in various scenarios. We demonstrate that plaquette states seem to naturally provide the correct stripe filling fractions.

I. INTRODUCTION AND OUTLINE

Throughout this paper we aim to address questions concerning planar and linear (stripe) filling fractions of doped Mott insulators by trying to see how much may be gleaned by mapping such systems onto spin models. The answers that we find depend greatly on the the assumed form of our constituent particles (single holes, pairs) and their various geometries (plaquettes, rungs, bonds). We will demonstrate that plaquette states seem to naturally provide the correct stripe filling fractions. By mapping onto spin models, we will also be able to examine various competing orders. Amongst other things, we will demonstrate (not unexpectedly) that in the limit of large on-site repulsions $U$, magnetic and superconducting orders always compete.

The outline of the paper is as follows. In Section(II), we lay out the general standard model of Doped Mott Insulator which will form the focus of our discussion. In Section(III), we examine the problem of spinless and spinful particles in the plane by a mapping to a spin model. We will see, in a special yet general set of models another rigorous example of the competition between magnetic and superconducting orders. Within these spin models that result for large U, we illustrate how magnetic order as well as the physically transparent number order (both portrayed by $\mathcal{S}_z$ in two different spin representation) compete with the dual superconducting order encapsulated by bilinears in the planar $\mathcal{S}_\perp$ multiplied by exponentials in of a topological nature.

In Section(IV), we map a model of hard core bosons (hole pairs) in non-overlapping plaquettes with arbitrary finite range interactions and hoppings onto a planar XXZ model. We find that if the physics is indeed dominated by such attractive pair states then, within the ground state, the average hole occupancy per site within the optimal doped state may be 1/4. The large deviation from the observed optimal doping in most doped Mott insulators is hardly surprising and points to the inadequacies of looking at attractive plaquette pairs alone within the plane: not unexpectedly, an analysis of the cuprates based solely on notions of doped Mott insulators and concurrently assuming only Bose pairs of the plaquette size might be flawed.

We next examine, in Section(V), plaquette pairs on bond-centered stripes and find, under a variety of circumstances, near 1/4-filling. We discuss the possibility of phase separation or modulation of the hole pairs along the bond centered stripe. When we relax the condition that diagonal pairs do not have to be in non-overlapping plaquettes, we will find, in the large hopping amplitude ($t$) limit, a 1/3-filling fraction of stripes. Higher and similar filling fractions are found for pairs on single rungs and legs. From this simple exercise we conclude that bond centered stripes cannot, perhaps, be described by simple pairs roaming the stripe axis, and that if pairs indeed do dominate the asymptotic low energy stripe scale physics as we suggested in an earlier paper [1], then they must be effectively confined to non-overlapping plaquettes in accord with pictures suggested by the DMRG calculations of White and Scalapino [2].

We proceed with a similar analysis of fermions on bond centered stripes (Section(VII)), and find that these lend themselves to near 1/4 filling. Our description fortifies earlier work by Nayak and Wilczek [3].

II. THE MODEL

We will focus our attention on the relatively standard model of doped Mott insulator, the extended Hubbard model:

$$
H = - \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{ij} V_{ij} n_i n_j,
$$

where $c_{i\sigma}^\dagger$ creates an electron on site $i$ with spin $\sigma$ and $j$ is a nearest neighbor of $i$. This model contains both
the movement of the electrons (hopping) \((t, \text{ kinetic energy})\) and the interactions of the electrons if they are on the same site \((U, \text{ potential energy})\). The Mott insulating nature is captured by this on-site repulsion which greatly inhibits hole motion. We have added an additional term representing all possible number-number interactions (of all ranges); these may be result from myriad interactions- e.g. Coulomb repulsions, interactions mediated by phonons. The number occupancy

\[
n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}, \\
n_i = \sum_{\sigma} n_{i\sigma}.
\]

As well known, in the infinite \(U\) limit, trivial spin-charge separation occurs in any dimension. The charge degrees of freedom may be trivially encapsulated by spinless degrees of freedom. For a review of this principle, the reader is invited to read Appendix(A).

At large \(U\), the extended Hubbard model of Eqn.(1) may be related to an extended t-J model,

\[
H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) + \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_{ij} V_{ij} n_i n_j,
\]

where \(\vec{S}_i = \sum_{\sigma, \sigma'} c_{i\sigma, \sigma'}^\dagger \vec{\sigma}_{\sigma, \sigma'} c_{i\sigma', \sigma'}\) is the spin of the electron at site \(i\), \(\vec{\sigma}\) are the Pauli matrices, and there is a constraint of no double occupancy of any site \(i\) \((n_i = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma}\) has expectation values 0 or 1). The reduction to a Hilbert space where no doubly occupied sites occur (the Gutzwiller projection) will be automatically incorporated in all things to come.

### III. COMPETING ORDERS FOR FERMIIONS IN THE PLANE

#### A. Spinless Fermions- A Competition between Charge And Superconducting Orders

With possible applications to the limit of infinite on-site repulsion \((U)\) in mind, we now examine the competition of charge and superconducting order within the plane. All that we will detail below can be derived straightforwardly. We take a slightly longer route in order to highlight the simple similarities between spin and charge when looked at through the prism of the Jordan-Wigner representation of \(S=1\) and \(S=1/2\) problems respectively. Although not of any use for most practical applications, a high dimensional Jordan Wigner transformation has been devised by Fradkin [4], and later extended by Eliezer and Semenoff [5]. Very nice novel extensions to various spinful cases were recently advanced by Batista and Ortiz [6]. The basic message is that the classic Jordan-Wigner [7] transformation rigidly linking spinless fermions and \(S=1/2\) spins in one dimension can, quite naturally, be extended to higher dimensions. The only complication is that now the kink operators that code for the statistics transmutations become high dimensional topological objects. To be more precise, the standard one dimensional string operator appearing in the usual Jordan-Wigner transformation is replaced by its more general counterpart

\[
K_j = \exp[i \sum_k \theta(\vec{k}, \vec{j}) n_k],
\]

with \(\theta(\vec{k}, \vec{j})\) the angle between \((\vec{k}, \vec{j})\) and a fixed ray (in the one dimensional case the “angle of site” \(\theta\) reduces to either \(\pi\) (for \(j < k\)) or zero (for \(k \geq j\)) leading to the standard string operator). In terms of these new kink operators, the Jordan-Wigner transformation then reads

\[
S_j^+ = c_j^\dagger K_j,
\]

\[
S_j^- = K_j^\dagger c_j,
\]

\[
S_j^z = n_j - 1/2.
\]

The simple pair operator \(\Delta_{ij} = c_j^\dagger c_i^\dagger\) may be expressed in terms of the spin variables. In the aftermath, we find that the superconducting pairing operator may be expressed as a product of kink variables with the XY components of the spins: \(S_j^x\) and \(S_j^y\). The incompatibility of charge \((n\ or\ S_z)\) and superconducting phase \((\text{descendant from} \ \vec{S}_i)\) orders is trivially reflected from the non-vanishing commutator

\[
[S^x, S^\pm] = \pm S^\pm.
\]

Explicitly, inverting all matters to the spin representation,

\[
c_j^\dagger = S_j^+ K_j^{-1} = S_j^+ \exp[-i \sum_{\vec{r}} \theta(\vec{r}, \vec{j}) S_{\vec{r}}],
\]

the commutator

\[
[n_k, \Delta_{ij}] = (\delta_{ik} + \delta_{jk}) \Delta_{ij},
\]

which is compatible with \(\Delta_{ij} = \exp[i(\phi_C^j + \phi_C^i)]\), and \(n_k = \frac{-i}{\partial \phi_C^k}\) with \(C\) denoting charge.

If Eqn.(1) captured all of the physics, then computing optimal doping would amount to the determination of the value of \(\langle S_z \rangle\) when we aim to maximize the topological pairing order parameter \(\Delta\).

#### B. Spinful Fermions- A Competition between Magnetic and Superconducting Orders

Just as in the spinless case, the simple summation relations that we will soon derive can be immediately
seen by direct computation (no Jordan-Wigner transformations are necessary). Nevertheless, in order to highlight the similarities between the charge and spin sectors as doublet (S=1/2) and triplet (S=1) representations of similar entities we will employ the Jordan-Wigner representation once again. Batista and Ortiz [6] extended the Jordan-Wigner transformations to spinful fermions. The operator
\[ \tau^\dagger_{j\sigma} = c^\dagger_{j\sigma}(1 - n_{j\sigma}), \]
along with its conjugate, may be transformed into spin S=1 operators in much the same way as for the spinless case. We note that within the large U limit, \( \tau^\dagger_{j\sigma} \rightarrow c^\dagger_{j\sigma}. \)

Any Hamiltonian in \( \{\tau^\dagger_{j\sigma}, \tau_{j\sigma}\} \) has the Gutzwiller (no double occupancy) projection automatically built into it. The general t-J Hamiltonian of Eqn.(3) will undergo no change when expressed in terms of \( \{\tau^\dagger_{j\sigma}, \tau_{j\sigma}\} \) instead of \( \{c^\dagger_{j\sigma}, c_{j\sigma}\}. \)

The transverse (XY) components of the spin may be written as [6]
\[ S^\dagger_j = 2^{1/2}(\tau_{j\sigma,+}K_j + K^\dagger_{j\sigma}\tau_{j\sigma,-}). \]

The z-component of the spin transforms as the on-site magnetization,
\[ S^\dagger_{jz} = \tau_{j\sigma,+} - \tau_{j\sigma,-}, \]
with \( \tau_{j\sigma} = \tau_{j\sigma,\tau_{j\sigma}}. \) As before,
\[ K = \exp[i\sum_k \theta(\vec{k}, \vec{j})\pi_k] = \exp[i\sum_k \theta(\vec{k}, \vec{j})(S^\dagger_k)^2], \]
where the, new, second equality follows from Eqn.(11) and the inbuilt constraint of no double occupancy. When we employ the inverse transformation, we find that \( \Delta_{ij} = c^\dagger_{i\sigma}c^\dagger_{j\sigma-\sigma} \) contains, similar to the case before, the transverse components of the spin \( S^\dagger_k \) multiplying topological operators \( K^{-1} \), which are simple exponentiated products in \( \{(S^\dagger_k)^2\}. \) Once again the non-commuting character of the spin components (Eqn.(6)) disallows concurrent ideal magnetic and superconducting orders. Explicitly,
\[ [S^\dagger_k, \Delta_{ij}] = -\frac{1}{2}(\delta_{ik} - \delta_{jk})\Delta_{ij}. \]

This is compatible with
\[ S^\dagger_k = \frac{i}{2} \frac{\partial}{\partial \phi_k^M}, \]
\[ \Delta_{ij} = \exp[i(\phi_i^M - \phi_j^M)], \]
with the superscript \( M \) denoting “Magnetic”. Trivially,
\[ [S^\dagger(\vec{q}), \Delta(\vec{p})] \neq 0, \]
with \( \vec{q} \) and \( \vec{p} \) arbitrary wavenumbers.

Examining Eqs.(8,13), we note that, apart from an important minus sign, magnetism competes with superconductivity in much the same way as the charge (number) field competes with pairing for spinless fermions. This is, of course, not all too surprising. We merely wished to highlight the similarities between the spin and charge sectors as S=1 and S=1/2 representations of a similar problem when viewed through the Jordan-Wigner transformation.

All of what we detailed henceforth was for singlet pairing. For a hypothetical triplet pair operator \( \Delta^{(i)}_{ij} = c^\dagger_{i\sigma}c^\dagger_{j\sigma} \) the commutation relations are trivially identical to those of the number and pairing correlations of Eqn.(8),
\[ [n_k, \Delta^{(i)}_{ij}] = \frac{1}{2}(\delta_{ik} + \delta_{jk})\Delta^{(i)}_{ij}. \]

To summarize, in a well known simple rubric,
\[ \text{[Spin, Pairing] \sim [Charge, Pairing] \neq 0.} \]

We further reiterate that the charge and spin sectors can be viewed as a doublet (S=1/2) and triplet (S=1) representations of similar entities. The spin component \( S_z \) takes on different roles the two different Jordan-Wigner transformations. This is simply yet another way of viewing matters. The similarity between the two sectors is highlighted in the SO(5) theory of S. C. Zhang [8].

IV. PLANAR PLAQUETTE PAIR STATES

Much of our approach henceforth was inspired by the beautiful work of Altman and Auerbach [10]. Let the operator \( \Box^\dagger \) denote the creation operator of a hole pair on a plaquette. The difference between pairs in the cuprates and in conventional BCS superconductors is that within the cuprates the pair size is very small which allows us to consider a reduction to plaquettes. This is also seemed to be supported by numerical calculations.

A. Mapping To An XXZ Model

Employing the Matsubara-Matsuda transformation [11] (trivially valid in any dimension)
\[ S^\dagger_i = n_i - \frac{1}{2}, \]
\[ S^\dagger_i = \Box^\dagger_i, \]
\[ S^\dagger_i = \Box_i, \]
we may map the most general Hamiltonian describing pair motions and interactions of all ranges
\[ \tilde{H}_{eff} = -\sum_{(ij)} \epsilon_{ij}(\Box^\dagger_i \Box_j + \Box^\dagger_j \Box_i) \]
\[ + \sum_{(ij)} V_{ij} n_i n_j + J^\dagger \sum_i \Box^\dagger_i \Box_i + ..., \]
(19)
tential \( V_{ij} \) allows (and favors) regions of different phase densities (i.e. phase separation).

**C. Superconducting Correlations, vortices, And A Numerical Value For Optimal Doping For Attractive Interactions**

Whenever the expectation value \( \langle S_\perp \rangle \) vanishes we immediately find half a pair per plaquette or, equivalently, a doping of quarter of a hole per site. In order to make the XXZ model maximally superconducting, we would like to make the order as XY like as possible to avoid phase separation into bosonic hole pairs. If we indeed impose from the outset the absence of \( Z_2 \) like order for the number operator \( S_z \) we find a quarter of a hole per site

\[
\delta_{\text{optimal}} = 1/4. \tag{21}
\]

The largest \( S_z \) (or number) fluctuations \( \langle (S_z - \langle S_z \rangle)^2 \rangle \) occur about the symmetric point \( \langle S_z \rangle = 0 \). This feature is far more generic than assuming a special model of two dimensional hard core bosons (as we have above). In high enough dimensions, the maximal fluctuations at the symmetry points may diverge signaling a critical point. Large number fluctuations enable well defined superconducting phase (XY) order. A trivial bound on XY order reads

\[
\langle S_\perp^2 \rangle \leq S(S + 1) - \langle S_z \rangle^2. \tag{22}
\]

As the number operator is the dual disorder operator for the phase, in order to have maximal phase ordering, we wish to avoid vortex like number expectation values. A finite number density \((n - 1/2)\), is analogous to a finite vortex density. This, in turn, is equivalent to an imposed external background magnetic flux density in a Josephson junction array. Non-uniformities in the charge order act as frustrating vortices. For maximal phase ordering we need to minimize the appearance of vortices. This entails lowering the effective magnetic flux background that spontaneously generated vortices must cancel.

Another way of viewing matters at very low finite temperature (like a low temperature classical model) is as follows: If \( J^2 \) were zero then adding an additional field \( h' \) would corrupt the XY order- the previous classical ferromagnetic XY ground state \( \vec{S}_\perp = (\cos \phi, \sin \phi) \) with the phase \( \phi \) uniform over the entire plane. Now imagine turning on \( J^2 \) and making it negative (attractive interactions amongst pairs). This will only further corrupt the XY order.

The relatively large deviation of the optimal doping found in the cuprates from 1/4 suggests that we may not easily view these doped Mott insulators at optimal or near optimal doping as merely composed of pairs of the plaquette size with attractive interactions.
These plaquette pair states are indeed the states observed numerically. Moreover, as emphasized by [10] they naturally display $d$-wave symmetry.

As before, we may use the operator $\Delta_{ij}^\dagger$ to denote the creation operator of a hole pair on a plaquette and subsequently employ the Matsubara-Matsuda transformation without change to obtain once again Eqn.(29).

As seen in Fig.(2), adding a hole pair along the bond centered stripe removes energetic ferromagnetic bonds. Such an effect will only serve as a weak sink favoring more hole pairs to drift into the stripe.

If the charge-charge interaction,

$$\sum_{ij} V_{ij} n_i n_j - 2 J \sum_i n_i$$

is repulsive for all $|i-j|$ (i.e. $V_{ij} > 0$), then in the extended spin model we will find exchange constant $J_z > 0$ for all $|i-j|$. A positive $J^z$ favors charge neutrality $\langle S_{tot}^z \rangle$ when the background charge of (-1/2) (if $\sum_j V_{ij} = 2 J$) is taken into account. For an attractive potential $V_{ij} < 0$ leading to $J_z < 0$, there is viable ferromagnetic order. The potential $V_{ij}$ allows (and favors) regions of different phase densities (i.e. phase separation).

In the presence of a vanishing electronic chemical potential

$$\mu = \sum_j V_{ij} - 2 J,$$

or, effectively, an external magnetic field $\tilde{h}$ of a similar magnitude, there is no spontaneous symmetry breaking in the XXZ chain

$$\langle S_z \rangle = 0$$

and there is an average of one pair per two plaquettes or a quarter of a hole per site. This is indeed in accord with experimental observations [13] and the numerical calculations of White and Scalapino [2]. In reality, the chemical potential albeit small compared to $t$ is not zero and a small deviation from 1/4 will be found. Nothing is inserted by hand here- the occupancy is dictated by the chemical potential (or magnetic field) which is finite yet may small compared to $t$ by virtue of the various parameters that it includes (i.e. $J/t$ and $\frac{1}{2} J \sum_j V_{ij}$). At its very core, the unbroken spin rotational symmetry corresponds to particle-hole symmetry trivially present at $\mu/t = 0$. This symmetry is lightly lifted by a small finite chemical potential shift relative to its vanishing value the particle-hole symmetric point.

We will later on demonstrate that if we assume only symmetrized rung states for each of the individual holes

FIG. 2. The DMRG calculation of the $t$-$J$ model by White and Scalapino. This and similar calculations typically employ open or cylindrical boundary conditions.

V. PLAQUETTE STATES ON STRIPES

The stripe constitutes a small system coupled to a large bath (the ambient antiferromagnet) from which it can draw holes. Depending on the chemical potential of the stripe, different hole densities will result. For ease we will invoke a simplifying yet non-essential assumption: by virtue of the large kinetic scale, the hopping amplitude $t$ is much larger than all potential effects, i.e. $\sum_j V_{ij}$ and the magnetic alleviation energy (the energy gained by removing bad ferromagnetic bonds along the seam of the stripe) $J$. With such assumptions, the chemical potential trivially vanishes. In reality, due to the finite corrections of both effects we expect the chemical potential $\mu/t \approx 0$.

As we will show assuming the constituents of the stripes to be of different geometries and nature (e.g. hole pairs on non overlapping plaquettes, diagonal or parallel hole pairs) different filling fractions will be found at the approximate particle-hole symmetric point $\mu = 0$.

We will now require that every two consecutive rungs of the ladder form a unique plaquette (such that these plaquettes do not overlap) and consider all possible pair states within these plaquettes.

As we will now show, if the chemical potential is indeed small by comparison to the kinetic hopping amplitude $t$, then assuming pair states in non-overlapping plaquettes will lead to the “correct” filling fraction. By “correct”, we allude to the coincidence, within the large $\mu/t$ limit, with the filling fraction attained from an original large $U$ Hubbard Hamiltonian for single fermions augmented by all possible hoppings and interactions amongst the holes.

As we show in section(VII B), if we start from the original Hubbard model and allow holes to do anything that they wish from there (e.g. remain single, pair, phase separate) we will find that the net hole filling fraction is 1/4. This coincidence suggests that plaquette pair states are indeed viable candidates for the pairs states populating bond centered stripes. Moreover, both numerical [2], and mean field [12] calculations lead to quarter filling as well as experimental data [13].
then no matter how the holes interact and whether they form pairs, phase separate, or not, a bond centered stripe must be nearly quarter filled when the chemical potential for the insertion of a hole is very small by comparison to the kinetic hopping scale $t$.

To conclude, in the final analysis, we expect

$$\delta_{\text{stripe}} \approx 1/4,$$  \hspace{0.5cm} (26)

where the approximation sign signifies the relatively small (compared to $t$) chemical potential shift due to magnetic alleviation energies and hole-hole interactions.

### VI. NON PLAQUETTE PAIR STATES

Here we show that unless the fundamental pair building blocks are not chosen properly then the hole density may come out to be incorrect (when contrasted with the very general single hole problem for consistency in the large $t$ limit). The filling fraction will be larger than a quarter found for the general hole problem before assuming anything about the possibility of pairing, phase separation etc. amongst holes. We will now analyze diagonal pairs which may be symmetrized and anti-symmetrized. Apart from some trivial numerical modifications, the considerations that we present here may be repeated word for word for “vertical” pair states extending along the rungs or “horizontal” pairs extending along the legs. There is a viable link between the correct symmetry of the pair state and its extension over different non-overlapping plaquettes and the anticipated hole density. In order to exhibit this link and point to the viability of plaquette pair physics, we will purposefully, focus on a pair state ansatz that will give an incorrect filling fraction in the $\mu/t \to 0$ limit. More complicated and comprehensive treatments may employ much of what is known about the two leg ladders (for instance, the SO(8) symmetry present in their low coupling limit [14]).

#### A. Diagonal Pairs

We will now write down an effective one dimensional model for diagonal pairs of two possible chiralities (left/right tilting) as shown in the right and left hand panels of Fig.(3). To give the reader a flavor of where we are heading the general argument may be summarized as follows- we will effectively make an exact projection of the two rung ladder along its axis to produce an effective one dimensional model. Henceforth we will denote the two natural diagonal pair chiralities (or polarizations) by a Greek index $\alpha = 1, 2$ and further employ the shorthand

$$\Delta_i^{(\alpha=1)} = c_{i,i+1,\sigma}^{\dagger} c_{i,i+1,-\sigma}^{\dagger},$$

$$\Delta_i^{(\alpha=2)} = c_{i,i+1,-\sigma} c_{i,i+1,\sigma}.$$  \hspace{0.5cm} (27)

for the hole pair annihilation and creation operators of the diagonal polarization of Fig.(3) ($\alpha = 1$) in terms of the electronic operators. In Eqn.(27) the first subscript (which is always one or two) marks the location of the hole on the ladder- on which of the two rungs it is found (upper or lower) while the second ($i$) denotes the location of the hole along the stripe (ladder) axis. The pair creation operator removes two electrons and the pair annihilation operator creates two electrons. Note that in these operators, there is no spin index symmetrization/anti-symmetrization. The spin polarizations are dictated by the location along the ladder (whether or not $i$ is even. We may conform to the convention that the spin subscript $\sigma = \uparrow$ if $i$ is even and that $\sigma = \downarrow$ along the odd rungs (i.e. we will choose our origin $i = 0$ in such a way that the spin polarization of both electrons on that rung is $\sigma = \uparrow$). The introduction of each diagonal pair states removes two bad magnetic bonds along the two rungs that it occupies.

The number associated with these hole ("h") pair operators is, as usual,

$$n_{i,h}^{(\alpha)} = [\Delta_i^{(\alpha)} \dagger \Delta_i^{(\alpha)}].$$  \hspace{0.5cm} (28)

We therefore can write the most general effective one dimensional Hamiltonian

$$\hat{H}_{eff} = - \sum_{(ij)} \tilde{J}_{ij}^{\alpha \beta} \Delta_i^{(\alpha) \dagger} \Delta_j^{(\beta) \dagger} + \Delta_i^{(\beta) \dagger} \Delta_j^{(\alpha) \dagger} + \sum_{(ij)} V_{ij}^{\alpha \beta} n_{i,h}^{(\alpha)} n_{j,h}^{(\beta)} + \tilde{J}' \sum_{i,\alpha} \Delta_i^{(\alpha) \dagger} \Delta_i^{(\alpha)} + \ldots$$  \hspace{0.5cm} (29)

where the ellipsis denote higher order terms in $\{\Delta_i\}$. All potential terms appear here including ones with infinite long range interactions (e.g. Coulomb effects) in which terms like $V_{ij}$ decay as slowly as desired as a function of the separation $|i - j|$. Note that as a single hole cannot be doubly occupied (or an electron of fixed spin cannot be twice removed), no two diagonal bonds may share the same site; this may formulated in terms of an effective infinite hard core repulsion: $V_{i,h}^{\alpha \beta} = V_{i+1,h}^{\alpha \beta} = \infty$.

Employing the Matsubara-Matsuda transformation once again we arrive at a flavored version of Eqn.(29) where we dress the various spins by the polarization (diagonal orientation of the pair that they represent). Insofar as commutators are concerned, the two polarization sectors are completely decoupled. Setting, for each $\alpha$, $\Delta_i = S_i^-$ and $\Delta_i^\dagger = S_i^+$, we see that the pair creation-and annihilation-operators form an SU(2) spin algebra. The effective Hamiltonian is a trivially flavored version of Eqn.(20):

$$\hat{H}_{eff} = - \sum_{(ij)} \tilde{J}_{ij}^{\alpha \beta} \Delta_i^{(\alpha) \dagger} S_j^{(\beta)} + S_i^{(\alpha) \dagger} S_j^{(\beta) \dagger} \Delta_i^{(\beta) \dagger} S_j^{(\alpha) \dagger} + \sum_{(ij)} \tilde{J}_{ij}^{\alpha \beta} S_i^{(\alpha) \dagger} S_j^{(\beta) \dagger} - \tilde{J}' \sum_{i,\alpha} \Delta_i^{(\alpha) \dagger} \Delta_i^{(\alpha)} + \ldots$$
may assume the eigenvalues \{1, 0, -1\} corresponding to a \(2 \times 2\) patch of the ladder being electronically full, having one diagonal hole pair, and two having diagonal hole pairs. The symmetric combinations \(\{\tilde{S}_i\}\) satisfy \(SO(3)\) algebra with spin one. The net number of electrons is given by the total magnetization of the symmetric \(\langle \tilde{S}_{i,\text{tot}} \rangle\) component.

C. Restricted Symmetric Hole Pair State Basis

We will now make the physical assumption (fortified by our earlier analysis [1]) that only the low energy symmetric hole pair bonding states appear at low energies. Defining, within the restricted symmetric hole pair state basis,

\[
S_i^- = \frac{1}{\sqrt{2}} (\Delta_i^1 + \Delta_i^2) \equiv \Delta_i,
\]

\[
S_i^+ = \frac{1}{\sqrt{2}} (\Delta_i^1 + \Delta_i^2) \equiv \Delta_i^\dagger,
\]

\[
S_i^z = \frac{1}{2} [1 - 2 n_{i;\text{symm}}],
\]

we see that \(\tilde{S}\) satisfies \(SU(2)\) algebra with \(S = 1/2\) within the restricted symmetric bonding state space \(\prod_i \langle \Delta_i^1 \rangle^r |0\rangle\) with \(r_i = 0\) or \(1\), and where \(|0\rangle\) denotes the vacuum state in which no holes are present. The bosonic hole pair states fill up the ladder as the electronic orbital states do in the atomic and molecular systems. We may regard this as an effective Hund’s rule. At low hole filling fractions, only the low energy bonding states will be occupied. At high hole occupancies (in excess of half a hole per unit site), anti-symmetric anti-boding states will also appear and the full \(SO(4)\) algebra of the full blown unrestricted Fock space will raise its head.

Substituting Eqs.(32,33,34) into Eqn.(29) and omitting any terms containing anti-bonding operators (which will take us out of the restricted symmetric pair state subspace) an arbitrarily high polynomial in \(\{\tilde{S}_i\}\) will result identical to Eqn.(20). The hard core repulsion term \(V[n_i^{(\alpha=1)} n_{i+1}^{(\alpha=2)} + n_i^{(\alpha=2)} n_{i+1}^{(\alpha=1)}]\) transforms into an analogous hard core term \(V S_i^z S_{i+1}^z\) for the z-component of the spins (the distance between up spins cannot be smaller than two).

Such a hard core term may be interpreted from first principles. A state containing nearest neighbor symmetric bonding pairs is not normalized to one. To have normalization we must consider the correlated four hole state \(2^{-1/2} \sum_{\alpha=1,2} \Delta_i^{\alpha \dagger} \Delta_{i+1}^{\alpha \dagger} |0\rangle\). The reduced norm (probability) of the nearest neighbor bonding pairs vis a vis other bonding pairs is similar to having a large potential barrier.
D. One Third Doping And Beyond

Sans the hard core constraint, the model has its ground state at half filling (i.e. the density of up spins is a half); Whenever an XXZ model has a nearest neighbor hard core constraint (whenever the distance between up spins cannot be smaller than two), the density of up spins is equal to a third within the ground state [15]. A careful counting of the various diagonal pair states reveals that the hole occupancy within the stripe is expected to be 1/3 in the large $t$ limit. Repeating the same exercise for hole pairs along rungs and legs we arrive at similar large hole densities.

VII. SINGLE ELECTRONIC DESCRIPTION

A. Symmetric Rung States

In an earlier work [1], we have numerically obtained the single hole and hole pair energy spectrum on a stripe. Let us first restrict attention to the single electronic description. The states along the various rungs form resonant bonding states. We will now make the physical assumption (fortified by numerics) that only the the low energy symmetric (or anti-symmetric) hole rung bonding states appear at low energies. We will now consider the symmetric (anti-symmetric) smearing of a hole along the two legs of the rung. Defining, within the restricted symmetric hole rung state basis, the two operators

$$c_{i;\pm} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} c_{i}^{(\alpha=1)} \pm c_{i}^{(\alpha=2)} \end{pmatrix},$$

with $c$ the electronic annihilation operator, $\alpha = 1, 2$ now a leg index, and $i$ a rung label, it is readily verified that these operators satisfy disjoint canonical Fermi anti commutation relations: $\{ c_{i;\pm}, c_{j;\mp}^{\dagger} \} = \delta_{ij}$.

We will assume that the even parity symmetric bonding hole states are lower in energy and restrict ourselves to that basis. In the problem of physical relevance, $|t_{ij}^{\alpha=1, \beta=2}| \gg$ all other hopping amplitudes and the hole will quickly resonate between the two rungs of the ladder before inching its way along the ladder axis.

Once again, the hole states fill up the ladder as the electronic orbital states do in the atomic and molecular systems. We may regard this as an effective Hund rule. At low hole filling fractions, only the low energy bonding states will be occupied. At high hole occupancies (in excess of half a hole per rung of a bond centered stripe or a hole per plaquette in the cuprate plane), anti-symmetric anti-bonding states will also appear and the algebra of the full blown unrestricted Fock space will raise its head.

In what will follow shortly, we will treat the symmetric rung holes as spinless fermions. An average density of half a spinless fermion (the particle-hole symmetric point) per rung corresponds to a quarter hole per site.

We will consider the extended Hubbard model in the restricted basis of these low lying symmetric rung states.

B. The Ideal Spinless Fermi Gas

As we review in Appendix(A), within the general Hamiltonian Eqn.(1) in the limit of infinite on-site repulsion $U$, the charge degrees of freedom transform into those of a spinless Fermi system. In the bare Hubbard model, at $U = \infty$ the system reduces exactly an ideal (non-interacting) Fermi gas with a dispersion

$$\epsilon_k = -2t \cos k.$$  \hspace{1cm} (36)

For a non-interacting Fermi gas, the zero temperature occupancy

$$\langle n_k \rangle = \theta(\mu - \epsilon_k).$$  \hspace{1cm} (37)

If inserting a hole leads to no change in the energy balance then the chemical potential, by its very definition, vanishes. The energetics of the chemical potential acts as a Lagrange multiplier enforcing a certain average occupancy. The energy of adding or removing an electron is the same (zero) at a chemical potential $\mu = 0$. By particle-hole symmetry, at $\mu = 0$ the chemical potential lies in the middle of the band and the occupancy of the rung symmetrized spinless fermi particles is a half- and that of the holes is 1/4. The particle-hole symmetry of the kinetic energy band is dictated by the hermiticity of the Hamiltonian. In fact, even if the Hamiltonian included arbitrary long range hoppings $\{ t_r \}$ and reduced to the general form

$$H = -\sum_{ij} t_{ij} (c_i^{\dagger} c_j + h.c.),$$

in the infinite $U$ limit, then by hermiticity whenever the chemical potential is zero the Hamiltonian will be particle hole symmetric. In that case, the density of rung symmetrized spinless fermions will be a half, and the density of holes along the bond centered stripe will be 1/4.

If the addition of holes (or removal of electrons) leads to a reduction in the magnetic strain energy along the stripe then the chemical potential for the electrons is reduced (or, equivalently, that for holes, is increased). A removal of a bad bond along the rung leads to a lowering of the magnetic energy by $J$. Thus the hole chemical potential $\mu = J$ and the net, rung symmetrized, charge occupancy is given by an integral of $\langle n_k \rangle$. The hole density is $\langle (n_k/2) \rangle$. This expectation value (hole occupancy) changes slightly with temperature according to the evolution of the Fermi function.
It is worthwhile viewing this, one last time, in terms of unbroken spin rotational symmetry in an effective XX(Z) model.

We now apply the Jordan-Wigner transformation in order to arrive at XX(Z) model. As well known, the infinite $U$ Hubbard Hamiltonian trivially transforms into

$$H = -2t \sum_i (S_{i,x}S_{i+1,x} + S_{i,y}S_{i+1,y}). \quad (39)$$

An infinitesimal chemical potential leads to an additional small magnetic field coupling to $\sigma_z$. The absence of spin symmetry breaking in this trivial example (no $\sigma_z$ interaction appears in $H$) leads to the conclusion that the band is half filled (or that the hole density is 1/4).

This is immediately seen taking note of

$$S_i^z = 1/2 - c_i^\dagger c_i. \quad (40)$$

A vanishing $\langle \sigma_z \rangle$ for the XY Hamiltonian of Eqn.(39) leads to $\langle n_j \rangle = 1/2$. Related back to our original problem, this implies a quarter empty electronic bond centered stripe. This value is seen here to be dictated by an unbroken particle-hole symmetry.

If additional interactions next nearest neighbor pieces of the Coulomb and other interactions ($\sum_{ij} V_{ij} n_in_j$) and the magnetic energy alleviation energy $J$ are added to the Hamiltonian then the Hamiltonian for the spinless symmetrized holes readily transforms to a full blown XXZ model with

$$H = -2t \sum_i (S_{i,x}S_{i+1,x} + S_{i,y}S_{i+1,y}) + \sum_{i,j} V_{ij} S_i^z S_j^z / 2(1 - S_i^z / 2) - J / 2 \sum_i (1 - S_i^z / 2)
\equiv \sum_{i,j} [-J_\perp (S_i^z S_j^z + h.c.) + J_\parallel S_i^z S_j^z]$$
$$+ \sum_i h S_i^z. \quad (41)$$

We first note that if the electrostatic energy $V_{i,i+1}$ is such that it equals the magnetic alleviation energy $J$ then by the absence of spontaneous symmetry breaking in one dimension, $\langle S^z \rangle = 0$ and the bond centered stripe is quarter filled. If, hypothetically, $S^z$ would spontaneously develop a nonzero magnetization then this would imply that even if in an ensemble of stripes, the overall density of holes would be a quarter on average, different stripes in the ensemble would exhibit two different densities about that mean.

An imbalance between $V$ and $J$ leads to nonzero $h$ and to a finite value of $\langle S^z \rangle \neq 0$, a deviation from quarter filling on every stripe. In the above we took into account both the Coulomb and magnetic alleviation effects in one go.

In a very nice paper by Nayak and Wilczek [3] it was observed that 1/4 filling of a doped chain is indeed predicted from the Bethe ansatz solution of Lieb and Wu [16]. Some of the symmetries of the 1/4 filled point were noted. Here we emphasize that at low chemical potential, quarter filling not only coincides with symmetries, but is, in fact, a rigorous outcome of symmetry considerations. Here we also note that a finite magnetic alleviation energy of the holes amounts to a shift in the chemical potential. The approximate calculations employed earlier are not mandatory for the determination of the hole occupancy within the ground state; in order to account for magnetic effects, we may simply set the hole chemical potential $\mu = J$, and subsequently integrate the known ideal spinless fermi number density $\langle n_e \rangle$ up to that energy to obtain an exact result.

APPENDIX A: A REVIEW OF TRIVIAL SPIN CHARGE SEPARATION IN ANY DIMENSION IN THE LIMIT OF LARGE ON SITE REPULSION

Here we review trivial spin-charge separation within any Doped Mott insulator (of arbitrary dimensions) in the limit of large on site repulsion energy $U \rightarrow \infty$. Let $\psi_{\sigma_1,...,\sigma_N}(x_1,...,x_N)$ be an electronic or “hole” eigenstate of the general Hubbard Hamiltonian augmented by all possible higher order interactions (these may be sparked by electron phonon terms, Coulomb repulsions etc.) and all possible range hopping amplitudes $t, t', t'', ...$ etc.

Recall that, trivially, $\psi_{\sigma_1,...,\sigma_N}(x_1,...,x_N)$,

- is anti-symmetric by virtue of its electronic constituents: $\psi_{\sigma_1,...,\sigma_N}(x_1,...,x_N) = -\psi_{\sigma_1,...,\sigma_N}(x_1,...,x_N)$.

Note furthermore that exactly at the $U \rightarrow \infty$ limit,
- $\psi(x_i = x_j) = 0$ irrespective of the spin indices $\sigma_1,...,\sigma_N$. The reason for this nodal behavior is trivially opposite spin occupation is forbidden by a divergent on site penalty $U$, and parallel spin occupation is strictly forbidden by the Pauli principle. Also, at finite temperature the probability for having any two particles occupy the same state strictly vanishes.

If we invoke this nodal, hard core, condition, then we may now remove the on site Hubbard repulsion from the original Hubbard Hamiltonian to obtain a general translationally invariant spin independent Hamiltonian $H$. Herein lies the crux of the trivial spin charge separation at infinite $U$.

The most general solution to the Schrödinger equation $H|\psi\rangle = E|\psi\rangle$ satisfying the last nodal condition with a spin independent Hamiltonian $H$ (all terms apart from the on site interaction $U$ are spin independent) is

$$\psi_{\sigma_1,...,\sigma_N}(x_1,...,x_N) = \chi(\sigma_1,...,\sigma_N)W(x_1,...,x_N), \quad (A1)$$
and linear superpositions of such degenerate solutions, where $W$ is a solution to the Schrödinger equation. Here the trivial spin-charge separation is manifest.
Let us now impose the Fermionic statistics condition
\[ P_{\text{spin}}^{ij} P_{\text{charge}}^{ij} = -1 \quad (A2) \]
for all \( i \neq j \). Note that \( [P_{\text{spin}}^{ij}, H] = 0 \) as the Hamiltonian is spin independent. As \( P_{\text{charge}}^{ij} = -[P_{\text{spin}}^{ij}]^{-1} = -P_{\text{spin}}^{ij} \), the charge permutation operator also commutes with \( H \).

This implies the function \( W \) must satisfy
\[
P_{\text{charge}}^{ij} W(x_1, ..., x_i, ..., x_j, ..., x_N) = \alpha_{\text{charge}}^{ij} W(x_1, ..., x_j, ..., x_i, ..., x_N). \quad (A3)
\]

The identity \( [P_{\text{charge}}^{ij}]^2 = 1 \) implies that \( \alpha_{\text{charge}}^{ij} = \pm 1 \).

In general, the energy of a nodeless function \( W \) is expected to be lower. However, the charge degrees of freedom cannot be completely symmetric: if the spinor \( \chi(\sigma_1, ..., \sigma_N) \) is fermionic (completely anti-symmetric) then it must vanish identically for \( N \geq 3 \) particles for the spin \( S = 1/2 \) electrons. In any dimension, the effective Hamiltonian can now be written in terms of the charge only spinless degrees of freedom. If the Hamiltonian is particle-hole symmetric (as expected by hermiticity of the most general arbitrary range kinetic terms) then whenever the chemical potential vanishes (whenever the insertion of a hole and a particle both cost zero energy), the average ensemble density of the correct spinless charge only spinless degrees of freedom. If the Hamiltonian is particle-hole symmetric (as expected by hermiticity of the most general arbitrary range kinetic terms) then whenever the chemical potential vanishes (whenever the insertion of a hole and a particle both cost zero energy), the average ensemble density of the correct spinless charge degrees of freedom must be a half. If, for instance, in any dimension, all low energy physics could be captured in terms of spinless charge pair degrees of freedom \( W = F(\{\phi(x_i, x_j)\}) \) then in terms of these pairs, the ground state of the system would be half occupied.

The charge degrees of freedom encapsulated in \( W \) can be symmetric with respect to, at most, single pairs (and anti-symmetric within these pairs); a higher symmetry is ruled out by the impossibility of a spinor anti-symmetric in three and more spin \( 1/2 \) indices (spinons cannot be fermionic).

Let us now regress to one dimension. Here, hard core bosons cannot be distinguished from spinless fermions and different symmetry states of \( W \) are in fact degenerate at the \( U = \infty \) point. This degeneracy is lifted as \( t/U \) becomes arbitrarily small but finite. As \( U \) is extremely large but finite \( 0 = |\psi_{\sigma_i=\sigma_j}(x_i = x_j)| < |\psi_{\sigma_i=-\sigma_j}(x_i = x_j)| \ll 1 \) and local singlet correlations are generated.

It has indeed been established by one dimensional Bethe ansatz [17] that at infinite \( U \), the function \( W \) is a Slater determinant of single particle momentum eigenstates.

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