Original Research Article

Why Are Stripes So Narrow? Confinement of Holes and Pairing On a Stripe

In this article we demonstrate how narrow stripes and pairing follow from a single simple principle: a strong antiferromagnetic background forces injected holes to hop in steps of two such that they always remain on the same sublattice. When applied to a domain wall in an antiferromagnet, this simple effect naturally leads to a number of results. First, we demonstrate that the holes are immediately (exponentially) localized on stripes. Consequently, we show that the holes on a stripe favor the formation of pairs on neighboring rungs or sites. We recover in this way the well known pictures of stripes found by White and Scalapino by numerical Density Matrix Renormalization Group (DMRG) calculations. Throughout this work much emphasis is placed on the problem of a two leg ladder immersed in a staggered magnetic field.

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I. INTRODUCTION

It has been nearly three decades since the discovery of the high-T_c superconductors[1]. Although much has been learned since, there is still no satisfactory explanation of what causes the superconductivity. There is widespread agreement that it should be possible to describe the electronic properties of the square CuO_2 lattices by the two-dimensional repulsive Hubbard model. This well known model is given by

$$H = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{i\sigma} c_{j\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c^\dagger_{i\sigma}$ creates an electron on site i with spin σ and j is a nearest neighbor of i. This model contains both the movement of the electrons (hopping) (t, kinetic energy) and the interactions of the electrons if they are on the same site (U, potential energy). The Hubbard model is one of the simplest possible models of interacting electrons. The main problem is then finding the possible solutions of this model. This however has proven not to be an easy task. The Hilbert space of the model is too large for exact numerical solutions. Monte Carlo simulations have the minus sign problem. U is approximately equal to $8t$, so we are neither in an extremely strong, nor in a weakly interacting limit. Therefore, perturbation theory is of limited use. In order to get somewhere we therefore need to invoke simplifications. In this article the main assumption is that we assume that a lightly doped system displays sublattice order.

Stripes were first detected in cuprates[2] in the famous neutron scattering experiment of Tranquada and coworkers. Earlier theoretical approaches already predicted stripes before their experimental discovery[3,4]. Various aspects have been investigated by numerous works, e.g.,[5,6]. Notably, similar phenomena and viable physical underpinning may also appear in further unconventional (pnictide and other) superconductors different from the cuprates, e.g.,[6]. A plot of the incommensuration as a function of doping (the Yamada plot), which is a straight line from 0 to 0.125 doping with a slope of $1/4$[7], indicates that stripes may be quarter filled. DMRG calculations by White and Scalapino[8] have further indicated that the ground-state for stripes in the t-J model is approximately quarter-filled.

The question of why stripes are quarter filled is not, however, the only enigma surrounding stripes. Other questions that still need to be answered are for instancei: why they are so narrow? Are they insulators or metals? Are they bond-centered of site-centered? Are they superconducting? Is the conductivity perpendicular or along a stripe? Are they like $4k_F$ or like $2k_F$ density waves[9]? In an offshoot to this article we will detail a possible reason why stripes are quarter-filled.

II. OUTLINE

Throughout this work we will focus our discussion on the Hubbard model. Nevertheless, all that we will state can be applied to a wider range of models with additional longer range interactions and hoppings. We will assume from the outset that bond-centered stripes (stripes with the geometry of two leg ladders) form antiphase domain walls in the surrounding antiferromagnetic and demon-

strate how self consistent localized eigenstates and pairing follow from this assumption.

In Section (III), we introduce the sublattice principle which will form the backbone of our analysis. In order to streamline the quintessential physics, we will be brief in exposing this principle. For further details regarding the underpinnings of this principle, the interested reader may peruse Appendix A. Invoking the sublattice principle, we will show in Section (V) how exponentially localized wavefunctions will be found when we assume, self consistently, that stripes form antiphase domain walls. We will find that the transverse stripe scale is of the order of the lattice constant. What drives stripe formation in our picture are not confining magnetic string potentials, but a rather novel kinetic effect which we term *dynamical confinement*.

Once we establish, self consistently, that bond centered stripes form domain walls in the surrounding antiferromagnet, we will move in small steps towards examining further microscopics. As we will explain in Section (VI), we will consider a bond centered stripe engulfed by a surrounding antiferromagnetic region as a two leg ladder immersed in an external staggered magnetic field. We will then consider the problem of a single electron on a staggered empty two leg ladder (Section (VII)) which will facilitate the analysis of a single hole on an otherwise full staggered two leg ladder (Section (VIII)). Both problems will lead to similar results.

This will be followed by a similar analysis for a two electron system on an empty staggered ladder and the inverted problem of two holes on a full staggered ladder, in Sections (IX) and (X) respectively. The surprising conclusion is that in this case there is an essential difference between electrons and holes. Numerically, we find that for holes, pair states are slightly favored over single hole states although the correlations are very faint.

Having shown how narrow bond centered stripes with bound pair states emerge, in Section (XII) we fuse all of our finding together to reconstruct the real space DMRG pictures of White and Scalapino.

In Section (XIII), we will examine the effects of longer range Coulomb effects and additional longer range kinetic terms to show how much of our self consistent analysis can easily be fortified by the addition of such terms.

III. THE SUBLATTICE PARITY PRINCIPLE

The physics of holes and spins in two dimensions is a very complicated subject. In this article we will invoke the simplifying assumption that much of the low energy physics of holes in a strong antiferromagnetic background can be summed in a nutshell:

Holes can only move in steps of two.

This principle is equivalent to the omission of spin flips, waves, and string states. This sublattice parity principle is, of course, a gross oversimplification- the physics of hole motion in an antiferromagnetic is a fascinating and rich topic. Nonetheless, the low energy single hole dispersion curves (requiring careful extensive numerical work) coincide very well with those immediately following from this principle. For a review of this often overlooked principle, the reader is invited to read Appendix (A).

Stated in formal terms, the principle amounts to Z_2 order, which has lately been much discussed in the context of its viable destruction[10].

Many beautiful works exist on the subject of stripe formation and dynamics[11]. Hole dynamics on the stripe has been primarily addressed in terms of spinon-holon excitations, as in the works of Tchernyshyov and Pryadko[12]. In this article we do *not* assume that the elementary excitations are spinons and holons. Our approach is closer in spirit to the very interesting work of Chernyshev, White, and Castro Neto[13], which aim to answer the same fundamental questions concerning stripes. Their work examines the elementary excitations within the framework of the t-J_z model by examining retraceable paths of a hole out of the stripe into the surrounding antiferromagnet. We arrive at much of the same physics using the sublattice parity principle as our only guide. Our derivations are much more pedestrian yet physically transparent as compared to the detailed Green's function and numerical DMRG analysis carried out by these authors.

Many works place much emphasis on the string states created by hole motion or on kinks[14]. In our low energy analysis, there are *no string states*. For a discussion on how string states can be avoided and for a demonstration that they do not dominate the low energy physics, the reader is referred to Appendix (A). Similarly, the role of a domain wall in an antiferromagnet as an effective attractive potential for holes simply by the bad ferromagnetic magnetic bonds that they remove, and the careful interplay between string states and transverse and longitudinal hole kinetics is not what we consider here. A large body of literature complements our simple asymptotic low energy analysis.

IV. A BOND CENTERED STRIPE IN THE ANTIFERROMAGNET

Fig. (1) shows the system which we will be looking at. We will examine the anatomy of a bond-centered stripe in an antiferromagnetic background. As foretold, we will neglect spin-flips and assume the background to be a perfect Néel antiferromagnet. We will further assume that there is a phase-shift in the staggered antiferromagnetic order parameter as we traverse the stripe. This implies that there is a seam of ferromagnetic bonds between spins on the two different legs of the stripe. The ferromagnetic bonds will cost a lot of energy. However, introducing holes into the stripe will reduce this strain. The ferromagnetic bonds will turn out to be essential to explain the stability of stripes against "hole evaporation".

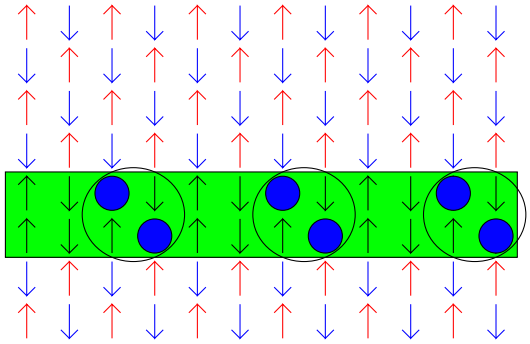

FIG. 1: Schematic representation of a quarter-filled bond-centered stripe in an antiferromagnet. We assume there are no spin-flips in the antiferromagnet. There is a π-phase shift in the staggered magnetization over the stripe. The cartoon above is not to be taken too literally. In reality, the pairs are smeared along the rungs.

In order to understand why a system would want to form such a stripe, we make the theoretical assumption that the system starts out with an antiphase boundary as shown in Fig. 2. Theoretically, one can force such a system by imposing suitable boundary conditions. If the system is L sites long, this will entail an energy penalty of, approximately, $2LJ_z$. Introducing holes into this system will reduce the energy of this ferromagnetic seam and ameliorate matters.

Topologically, stripes are not literally domain walls in an antiferromagnet (whose spins $\vec{S}$ are continuous variables and *not* Ising like) but rather topological excitations of the antiferromagnet known as skyrmions. As noted by Wilczek and Zee[15] and later incorporated by others in rather novel theories, e.g. Wiegmann[18], skyrmions in an antiferromagnet are cylindrical domains separating Néel states shifted by half a period. We note that topologically, stripes are identical to skyrmions stretched out to form domain walls spanning the entire lattice. Berry phase effects in the antiferromagnet associated with domain wall stripes can give rise to exotic statistics similar to that of skyrmions in 2+1 dimensions- as suggested by extending the results of[15] to our domain walls. Subsequent the initial appearance of our work[16], further illuminating investigations modeled magnetic order and fluctuations via an analysis of coupled two leg ladders[17].

V. DYNAMICAL CONFINEMENT (ON-STRIPE HYPOTHESIS)

We now examine what happens if we introduce a hole into the antiferromagnet with a domain wall (see Fig. 3). Once again, our major assumption still is that this hole moves in steps of two such that it will always stay on the same sublattice. We reiterate a note for the experts: our analysis has nothing to do with string states and kink (wiggle) motion beautifuly analyzed by many[12,13], and many of the works in[19–34] (our point of departure

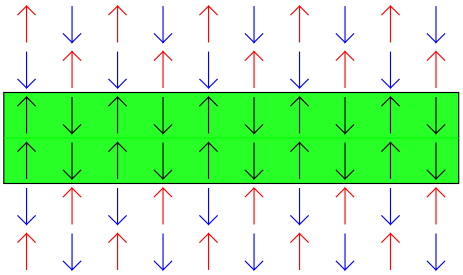

FIG. 2: We will make the assumption that the system starts out as antiferromagnetic with a "*domain wall*" - a skyrmion. We will analyze what happens if we add holes to this system.

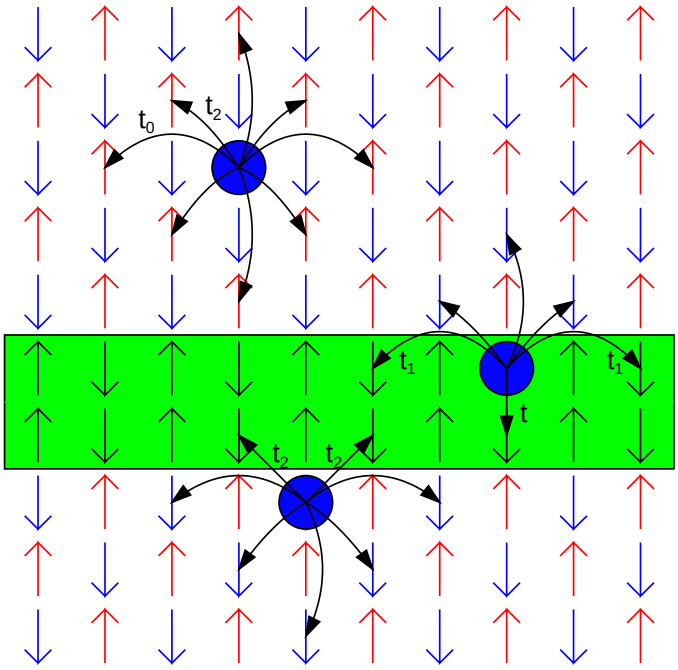

FIG. 3: A number of holes and an antiferromagnetic *domain wall* immersed in the surrounding antiferromagnet. We will show that the holes will automatically end up on the domain wall because of the single step up/down movement with an amplitude t which is possible within the domain wall (the stripe), but not in the surrounding antiferromagnet.

-the sublattice parity principle- is just a way to explicitly avoid high energy string states from the outset). Nor, does our bare analysis have anything to do with the role of the magnetic alleviation energies for a hole drifting into the stripe (whereby it removes bad ferromagnetic bonds) which plays the role of an effective attractive potential. Such effects will only enhance the bare findings that we report here.

With these remarks in mind, we note that if the hole is in the antiferromagnet, far away from the stripe, it has eight positions were it can move to (see Fig. 3). If it is sitting next to the boundary (just outside the stripe), it loses one hop, because of the reversed sublattice structure. The remaining seven hops are all the same as if the

boundary was not there.

Larger changes happen with a hole located within the stripe. For such a hole there are only six hops left. In Fig. 3, the hole on the stripe cannot move downward left or downward right because of the change in sublattice structure. So, naively, one might come to the conclusion that a hole has more kinetic energy in the antiferromagnet then if it is on or near the boundary/stripe. Naively, confinement of the hole in the stripe would cost kinetic energy. However, this is not the case.

The reason is that within the antiferromagnet the holes can only move in two steps longitudinally with an amplitude t_0 or diagonally with an amplitude t_2 which are of the order of $J = t^2/U \ll t$ (the uniniated reader is refered to Appendix(A) for an exposure to the origin of the exchange coupling J). On the stripe the hole can stay on the same sublattice by doing a single (instead of double) step up or down with amplitude t. As a consequence, the hole has a much larger kinetic energy if it is situated on the stripe. Therefore we find that the hole automatically drifts toward the stripe: the amplitude for the ground state wavefunction is maximal for sites on the stripe and decays exponentially the further the sites are away from the strip (see Fig. 4). Holes are driven by an increase in kinetic energy (not exchange energy) to the domain wall. We term this mechanism "*dynamical confinement*". The word dynamical is used because it is the motion of the holes on the stripe that lowers the energy. The primary role of kinetic energy in favoring the stripe as a ground state has been discussed many times before, e.g.[11–13]. Nonetheless, the trivial (yet sizable) lowering of the kinetic energy allowed by hole motion along the ferromagnetic rungs on the domain wall seems to have gone unnoticed.

For the two dimensional problem of a single hole in the vicinity of a full domain wall embedded in a surrounding antiferromagnet (of the variant shown in Fig. (3)), we may work in a very much reduced Hilbert space. In effect, the strongly correlated many particle system reduces to a single particle problem defined on half of the lattice. As there are, *ab initio*, four possible electronic states on each site (empty, one electron with its spin up, an electron with spin down, and an up and down electronic pair), the Hilbert space of an N site system is, trivially, of dimension 4^N. Invoking the sublattice parity principle allows us to reduce the Hilbert space to a mere size of $N/2$. The Hubbard Hamiltonian is then reduced to a purely kinetic model, having an amplitude t for nearest neighbor direct hops within the stripe, amplitudes t_0 and t_2 for longitudinal and diagonal two step hops (as depicted in Fig. 5 for the horizontal motions) within the antiferromagnet and an amplitude t_1 for two step hopping within the stripe along the axis of the ladder.

Before doing a more detailed analysis, let us first give the reader an intuitive feeling of where we are heading. Looking at Fig. (3), we note that a hole in the bulk disperses with an energy

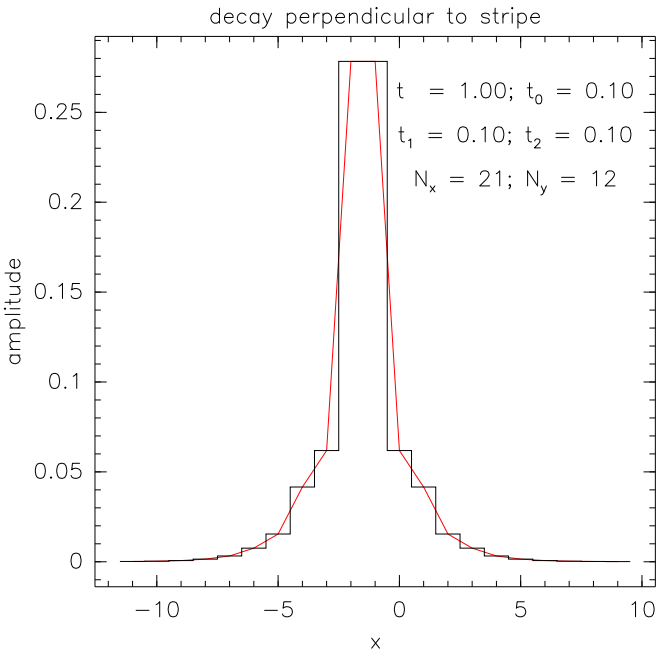

FIG. 4: Groundstate wavefunction perpendicular to a domain-wall for a single hole in an antiferromagnet. This was calculated using the simple approximation discussed in the maintext. The hole prefers to be on the stripe. We find $|\psi| \approx |\frac{t_0}{t}|^y$. The line in the figure just connects the midpoints. N_x and N_y are the linear extents of the two dimensional system and the hopping amplitudes t_0, t_1 and t_2 are as defined in Fig. (3).

$$\begin{aligned}\epsilon_{\rm bulk} &= \epsilon_0 - 2t_0(\cos 2k_x + \cos 2k_y) \\ &\quad -2t_2((\cos(k_x + k_y) + \cos(k_x - k_y)). \end{aligned} \quad (2)$$

Similarly, along the ladder,

$$\epsilon_{\rm stripe} = \epsilon_0 \pm t - 2t_1 \cos 2k_x, \quad (3)$$

where the second, $\pm t$, contribution denotes the energies of the bonding/antibonding states along the rung. Within this approximation, a sizable finite gap $\Delta \approx t$ separates the minima of both dispersions. In our analysis, it is this $\mathcal{O}(t)$ gap which is the main driving force for self consistent stripe formation having nothing direct to do with string states and magnetic alleviation energies (which are all of order $\mathcal{O}(J)$).

In reality, the hole can hop between the stripe and its surrounding bulk: the stripe states may be connected to the bulk. The low lying stripe states are however much lower in energy than their counterparts within the bulk. As a consequence, holes become localized on the stripe. As $t \gg t^2/U = \mathcal{O}(t_0) = \mathcal{O}(t_2)$, the on stripe dispersion is markedly lower in energy than its counterpart for motion within the antiferromagnet. This leads to an exponential decay of the lowest eigenstates states out of the stripe.

We have numerically diagonalized a 12 x 21 system with a direct nearest neighbor hopping amplitude $t = 1$, effective longitudinal and diagonal next nearest neighbor hopping amplitudes $t_0 = t_2 = -0.1$ within the antiferromagnet, and a next nearest neighbor amplitude along the axis of the stripe (ladder) $t_1 = -0.1$. The groundstate wavefunction is, to good numerical accuracy, given by

$$\psi(x, y) \approx |\frac{t_0}{t}|^y e^{ik_x x}. \quad (4)$$

Fig. (4) depicts this wavefunction along the direction perpendicular to the stripe. This figure is similar to Fig. 22 from Chernyshev *et. al.*[13] who calculated this from a 11×7 t-J_z system employing the numerical DMRG method. Our approach leads directly to this exponential confinement due to the *dynamical confinement*, without the need for complicated numerical calculations.

We will now aim to give the reader an intuitive grip on the physics along with the ability to easily derive rigorous bounds on hole localization within the planar problem.

If we were to allow a hole on the particle to hop to a larger number of neighbors within the bulk (i.e. to artificially enhance kinetic motions and lower confining tendencies), then we may map our system into the dynamics of pseudo-spin 1/2 particles in the presence of a transverse magnetic field. The mapping is as follows: let us mark each point within the bulk by its sublattice parity (up/down) number as depicted in Fig.(3). Let us now tile the plane into vertical 2×1 domino blocks lying with their long side parallel to the y axis. Each domino within the bulk contains one up and one down site; the labelling of the up and down sites on the dominos lying along the rungs of the ladders may be done arbitrarily. Next, let us envision replacing each domino by a single spin-1/2 particle: the number of the fictitious spin-1/2 particles is equal to half of the number of sites which we now label by m and n. For simplicity we will now assume that all second order hops are of equal magnitude σ. Let us now consider the Hamiltonian

$$H = -\sigma \sum_{\langle mn\rangle, d} (c^\dagger_{md} c_{nd} + c^\dagger_{nd} c_{md}) - \sum_{n \in ladder} \vec{h}_{ext} \cdot \vec{D}_n, \quad (5)$$

with the fictitious external magnetic field $\vec{h}_{ext} = t\sigma_x \hat{e}_x$ oriented along the transverse x-axis, and $\vec{D}_n$ the spin of the psuedo-particle (domino) along the n-th rung od the stripe and d is the pseudo-spin polarization label. In the first term m and n span the entire plane; the sum is performed over all nearest neighbor site $\langle mn\rangle$ and on four of the eight next nearest neighbor sites (such that all same sublattice hoppings of the holes within the bulk are accounted for). For holes not far from the stripe or on it, the Hamiltonian of Eqn.(5) introduces additional unphysical motions. These allow hoppings of the holes off and on the stripes which are disallowed- such additional terms can only enhance delocalization tendencies. The second term in Eqn.(5) codes for the nearest neighbor up/down hops along the same rung- these alter a pseudo-spin up state to a down state and vice versa. We trivially observe that the low energy dynamics corresponds to the motion of a $|\rightarrow\rangle$ particle polarized along the applied transverse field sensing an attractive confining potential of strength t along the stripe. In physical terms, the psuedospin polarized state $|\rightarrow\rangle = 2^{-1/2}(|\uparrow\rangle + |\downarrow\rangle)$ corresponds to the symmetric low energy bonding state (and its counterpart $|\leftarrow\rangle$ corresponds to the high energy antibonding state). The ground state is simply that of a polarized $|\rightarrow\rangle$ particle (the symmetric bonding state) sensing a well of infinite extent along one axis and having a finite extent ($2a$, with a the lattice unit) along the transverse direction. As the problem is translationally invariant along the ladder axis, the longitudinal momentum k_x is a good quantum number. The lowest lying wavefunction is translational invariant along the infinite cylindrical axis ($k_x = 0$) and, at long distrances, has the transverse profile of a particle of an effective mass $m_{eff} = 1/(2\sigma)$ subject to the influence of a potential well of depth t and width ($2a$). This trivially leads to an exponentially decaying amplitude in the direction transvserse to the stripe. As $t \gg J$, this confining tendency is much more profound (and physical) than most of the common magnetic bond (J) arguments prevalent in the literature. The reader should bare in mind that our point of departure- the sublattice parity principle is correct only as low energy scales (as compared to J). Nonetheless, what drives localization in our picture at low energy scale are the much more significant kinetic effects which outshadow the common bad bond (J) counting arguments.

The solution to this potential well problem is standard. Scaling back by a factor of two to the original (non-domino) coordinates along the $y-$ axis, we find, asymptotically,

$$\psi(x, y) \approx A \exp[-2\alpha|y|];\ |y| \gg a, \quad (6)$$

with the lowest lying bound state of Eqn.(5) is obtained by the solution of the transcendental equations

$$[\beta a \tan \beta a = \alpha a] \text{ and } [a^2(\alpha^2 + \beta^2) = \frac{1}{\sigma} t]$$
$$\text{or } [\beta a \cot \beta a = -\alpha a] \text{ and } [a^2(\alpha^2 + \beta^2) = \frac{1}{\sigma} t] \quad (7)$$

having the largest value of α.

Eqn.(6) gives an upper bound on the leakage of the "hole" wavefunction out of the stripe. If we set $\sigma = \max\{t_0, t_1, t_2\}$, we obtain a rigorous upper bound on $|\psi|$, at large distances $|y|$, consistent with our numerical findings (Eqn.(4)). As the Hamiltonian of Eqn.(5) contains additional unphysical hopping processes from the ladder to its environment, a localized state found for the Hamiltonian of Eqn.(5) implies even more localized states for the more restricted physical problem.

We may similarly address the problem of an arbitrary stripe configuration. In general, adding additional hoppings transforms the problem of the hole motion within

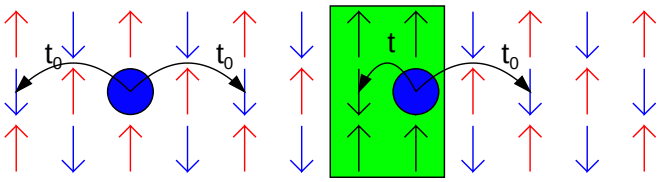

FIG. 5: One-dimensional example showing the reason for *dynamical confinement*. Outside the stripe, the hole moves in steps of two with an amplitude t_0. Inside the stripe it can make a direct hop with amplitude t with $t \gg t_0$.

and/or near stripes to a kinetic planar problem of a hole coupled by Zeeman couplings to magnetic fields piercing the plane along the stripe trajectories. A multitude of viable self consistent minima of narrow stripes of various geometries are found. Stripe dynamics is akin to the motion of the fields (solenoids) piercing the plane; these, in turn affect hole dynamics by a Zeeman like effect. The evolution of a hole-stripe system may be addressed via such a self consistent scheme.

A related way of immediately deriving lower bounds on the diffusion of the hole out of the stripe amounts to looking at the transverse cross-section of the stripe as depicted in Fig. (5), and examining single hole motions. Solving the Schrodinger equation for this one dimensional system, we immediately obtain a localized bonding state of the lowest energy. As here fewer hops are accounted for than in the original physical problem, the solution serves as a lower bound on "hole" wavefunction leakage out of the stripe. When fused with the previous upper bounds from the pseudo-spin system, we immediately obtain both lower and upper exponential bounds on asymptotic hole propagation out of the stripe.

In this scheme, splintering the sites according to their sublattice numbers (equivalent to the magnetic field sensed by a spin of definite polarization if it is placed at various locations throughout the lattice) introduces hopping parameters for the low energy dynamics with no potential energy in sight. As shown by our analysis, magnetic alleviation effects are not imperative for achieving this dynamical confinement (even when direct magnetic effects are removed we nunmerically attain exponential localization with little noticable change). We retiterate that we are examining the reduced Hilbert space where no magnetic string states exist from the outset.

In our approach, we first create an antiferromagnetic spin structure with domain walls and then dope the system. Then, if the spin structure is strong enough, the holes will migrate to the walls and will form a charge structure. Hopefully we have convinced the reader that sublattice parity order can indeed drive stripe formation. The energy scale associated with this discrete sublattice parity (Z_2) order[10] can indeed be quite high: the persistence of incommensurate peaks up to at least the high energy resonance peak in YBCO might be interpreted as an indication that the stripe presits to be a domain wall up to very high energy scales[35]. Experimentally, charge order is a far greater robust driving force for stripe formation than spin order. The role of sublattice parity (albeit its high energy scales) is not clear at the time of writing. The reader should consider our argument as a self-consistent one in which the creation of the no-hole domain-wall first is a theoretical device that simplifies theoretical discussion. Summarizing, we have seen that once there is a ferromagnetic seam in a very strong antiferromagnet, single holes will automatically move to this seam and be exponentially localized onto them. In the remaining part of this article we will see what the consequences are of this result for more than one hole on the stripe. The localization of the holes is in accord with NQR measurements, e.g.,[36].

VI. STAGGERED LADDER SYSTEMS

We have seen that by dynamical confinement we may consider an antiferromagnetic domain wall as a two-leg ladder with staggered boundary conditions. So, once again we can restrict our Hilbert space. Ladder systems have been extensively studied throughout the years. Hundreds of works on standard (unstaggered) ladder systems have been carried. For a well-known review see Dagotto and Rice[37].

In our case, the influence of the antiferromagnet surrounding the ladder is still there. The surrounding antiferromagnet effectively gives rise to staggered boundary conditions. In the up and coming, we will look at two-leg ladders with staggered fields mimicking the surrounding antiferromagnet. The staggered fields endow the ladder with a sublattice parity structure. Unfortunately, to date, staggered ladders have not been investigated intensively.

Krotov, Lee, and Balatsky[38] examined staggered ladders for the Hubbard model at small U. In this limit, one starts with a non-interacting system and then derives the renormalization group equations. Staggered spin ladders without any holes have been studied by Wang *et. al*[39]. However, staggered ladder systems with holes in the large U limit have not yet been addressed before as far as we know. We will now analyze staggered two leg ladders in a rather pedestrian manner. We verified the perturbative results that we will cite by explicit numerical computations.

VII. THE SINGLE ELECTRON ON AN EMPTY STAGGERED LADDER

To understand the effect of the boundary conditions on the movement of electrons and holes on the ladder we first examine a single electron on an empty ladder immersed in a staggered magnetic field. This is, of course, a hypothetical situation, but it is nevertheless a good starting point for our discussion. If the electron is on the correct sublattice (i.e. if its spin polarization is opposite

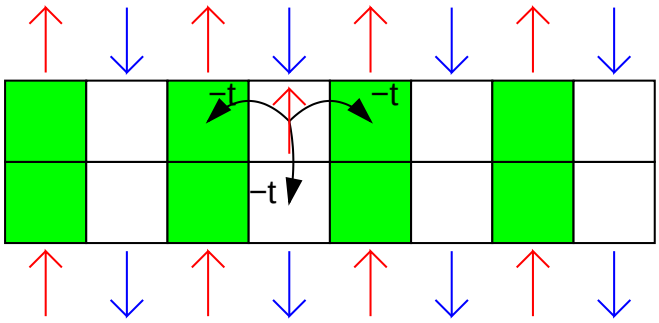

FIG. 6: Single electron on an empty ladder. In principle the electron can hop to all its nearest neighbors with an amplitude t. However, the ladder is embedded in an antiferromagnetic background that influences the electron on the ladder.

to that of the applied staggered magnetic field) then its magnetic energy will be $\epsilon_0 = -J$. Being on the wrong sublattice leads to a magnetic energy penalty of $\epsilon_1 = +J$.

This gives rise to staggered potentials on the ladder. The resulting Hamiltonian for the system as shown in Fig. (6), reads

$$H = \begin{pmatrix} \epsilon_1 & -t & -t & & & & & & \\ -t & \epsilon_1 & 0 & -t & & & & & \\ -t & 0 & \epsilon_0 & -t & -t & & & 0 & \\ & -t & -t & \epsilon_0 & 0 & -t & & & \\ & & -t & 0 & \epsilon_1 & -t & -t & & \\ & & & -t & -t & \epsilon_1 & 0 & -t & \\ & & & & -t & 0 & \epsilon_0 & -t & -t \\ & 0 & & & & -t & -t & \epsilon_0 & 0 & -t \\ & & & & & & -t & 0 & \epsilon_1 & -t \\ & & & & & & & -t & -t & \epsilon_1 \end{pmatrix}. \quad (8)$$

Here we express the Hamiltonian in terms of ordered real-space basis states where we place the upper and lower sites of each rung adjacent to each other. An electron at any site can always hop to three other sites. Because this is a single particle problem with a translational invariant potential (with unit cell of size two), the eigenfunctions of this Hamiltonian can exactly be determined. They are exactly given by

$$\psi = (B, \pm B, Ae^{ik}, \pm Ae^{ik}, Be^{2ik}, \pm Be^{2ik}, Ae^{3ik}, ...). \quad (9)$$

Here A and B are determined by

$$\begin{aligned} E_k &= \epsilon_0 \pm t - 2t\frac{B}{A}\cos k \\ E_k &= \epsilon_1 \pm t - 2t\frac{A}{B}\cos k. \end{aligned} \quad (10)$$

The energy can immediately be obtained from

$$\begin{Vmatrix} \epsilon_0 \pm t - E_k & -2t\cos k \\ -2t\cos k & \epsilon_1 \pm t - E_k \end{Vmatrix} = 0, \quad (11)$$

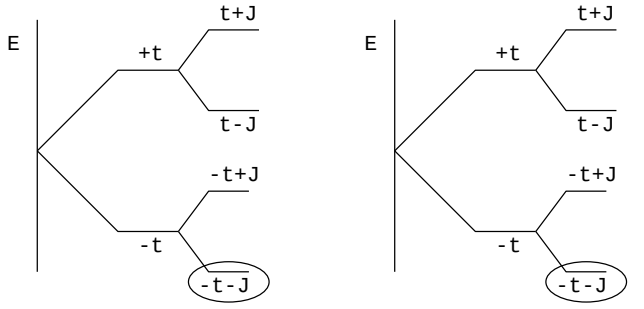

FIG. 7: Energy diagram for a single electron on an empty staggered ladder. If the staggered potential is large (large J), the splitting J is more important than t. In the lowest state, there are only $N/4$ states. These are the same states as for a single one dimensional model where an electron moves in steps of two. If $J \ll t$ (right) we still get the same lowest sector.

leading to

$$\begin{aligned} E_k &= \pm t \pm \sqrt{J^2 + (2t\cos k)^2} \\ &= \pm t \pm \sqrt{J^2 + 2t^2 + 2t^2\cos 2k}. \end{aligned} \quad (12)$$

This dispersion illustrates that, due to the staggered boundary conditions, the electron effectively moves in steps of two. Fourier transforming the energy shows that because of the symmetry between k and $\pi - k$, only terms which have an even number of steps from the starting point may have an amplitude unequal to zero: odd, sublattice parity interchanging, hops are banned. In more physical terms, this trivially corresponds to the halving of the period (in k) in the dispersion E_k.

Eqn. (12) shows that, for unphysically large $J \gg t$ (a strong influence of the surrounding two-dimensional antiferromagnet), the Hilbert space splits up in four different sectors. First, there is a splitting because of the boundary conditions: half of the sites have the electron on the right sublattice, which leads to a low energy of $-J$. The other half have the hole on the wrong sublattice, with an energy of $+J$. Because the upper and lower leg of the ladder are exactly equivalent, the electron will slosh back and forth between the upper and lower legs. This, in turn, leads to bonding/antibonding linear combinations of the upper and lower sites along each rung, further splintering the Hilbert space into two additional subsectors. The lowest sector, which contains $N/4$ basis states, consists of wavefunctions with the electron on the right sublattice (e.g. a spin up polarized electron on the up sublattice) with the symmetric linear combination (bonding) of upper and lower sites.

In the large J limit, Eqn. (12) simplifies to

$$E_k = -J - t - 2\frac{t^2}{2J} - 2\frac{t^2}{2J}\cos 2k. \quad (13)$$

Not surprisingly, we see that we this energy corresponds to the electron populating the correct sublattice

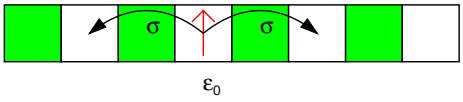

FIG. 8: Effectively, the electron moves on a one-dimensional chain in steps of two. There are only two effective parameters: the on-site energy ϵ_0 and the two site hopping amplitude σ.

$(-J)$ and being smeared along the two rungs in a symmetric bonding fashion $(-t)$. We can easily read off that the effective hopping is in steps of two from the $\cos 2k$ term. Because we are in the large J limit, the hopping amplitude in second order perturbation theory is given by $\frac{t^2}{2J}$. We have to hop twice (t^2) over an intermediate state with energy $2J$. The extra contribution $-2\frac{t^2}{2J}$to the energy comes from virtual excitations where the spin moves one position to the left or right and immediately returns back. There are two possible ways of doing this, and the amplitude again is $\frac{t^2}{2J}$. Thus, we can intuitively understand every term in this limit.

There is a gap of $2t$ separating the lowest Hubbard band from the antibonding states. Because $2t$ is a very large energy scale (approximately 0.5 eV, or 5000 K), we can neglect the influence of the other sectors and may restrict our attention only to the lowest sector.

Our discussion above hinged on the assumption that J is very big $(J \gg t)$. This assumption is not satisfied in the physically relevant region wherein $J \approx 0.25t$. In the physically relevant regime, we still have a splitting of the Hilbert space into four sectors (see Fig. (7)). The lowest Hilbert sector is still the same one as the one for the large J limit. For small values of J compared to t, the groundstate properties are still dominated by the $-J$, $-t$ sector. However, the low lying excitations out of the lowest sector are now to the sector where the electron goes to the wrong sublattice (a single hop) instead of going from a bonding to an antibonding state. Such hops will lead to string states. Nevertheless, as long as the width of the lowest Hubbard band is small compared to $2J$ (which itself is also a large energy, of the order of 2400K), we can still think in terms of bonding states on the correct sublattice. Within the lowest Hubbard sector, the electron will only be on the even lattice sites. Effectively, only second order hops are present. Because of the hybridization of up and down sites on a rung, it is sufficient to consider the one dimensional model shown in Fig. (8).

Just as for the single hole in the two dimensional antiferromagnet, discussed in Appendix (A), a lone electron on the empty ladder moves as an effective quasiparticle, with a sublattice hopping amplitude σ.

VIII. ONE HOLE ON A FULL STAGGERED LADDER

We now examine one hole in an otherwise full ladder immersed in a staggered external magnetic field. The single spin problem was very simple to solve analytically given our assumptions. The single hole problem is exceedingly more difficult because it is a strongly interacting many body problem. For a system of only 6×2 sites, there are already approximately $800,000$ states! Systems of this size and larger may be addressed by employing the Lanczos method of diagonalization, which only finds the lowest eigenstates of a matrix. We employed this method for systems of up to size 8×2. The complicated results that follow from this numerical study can be understood quite easily for large values of J. Though not the physically relevant regime, just as in Section (VII), both for $J > t$ and $J < t$, the ground state is in the same sector of Hilbert space.

For large values of J, the basic properties are once again those of a single quasiparticle. From the outside, we again assume that the hole cannot leave the stripe. An electron next to the hole can move to the position of the hole, leading to a string-state with one wrong spin. The hole can also move up and down. And it can move in steps of two to the left and right. In addition, we can have spin flips on the ladder. However, just as in the two-dimensional antiferromagnet we neglect the spin-flip processes. For large values of J we find once again a number of Hubbard sectors. The lowest sector has N/2 states where the hole is on the right sublattice and an energy of approximately $-2(N-1)J$. Above this lowest Hubbard sector we have the Hubbard sector with a string state of length one. There are 2N states in this sector. The gap between this sector and the lowest sector above it is $\Delta = 4J \approx 4800K$. We could ingnore this sector if this gap is large with respect to the internal splitting of the lowest Hubbard sector. This bandwidth is given by $4t''$ with $t'' = \frac{t^2}{U+4J} \ll t$. For $U \approx 8t$ we have $t'' \approx 0.1t$: both J and t have approximately the same amplitude. However, for the groundstate properties, the relevant properties are those of the lowest a single hole moving in steps of two. The band, shifted down by $t^2/2J$ by virtual hopping, has the dispersion of an inverted cosine. The gap $\Delta = t$, separating the on-stripe states from those in the surrounding antiferromagnet, is large with respect to t''. The spins adjust to surrounding antiferromagnetic. In the $U, J \gg 1$ limit,

$$\begin{aligned} \epsilon_0 &= -J - t - 2\frac{t^2}{2J}, \\ \sigma &= 2\frac{t^2}{U+2J}. \end{aligned} \tag{14}$$

The motion of a single hole on a stripe and its motion in a two dimensional antiferromagnet is identical. The only difference between the parameter sets, is sparked by

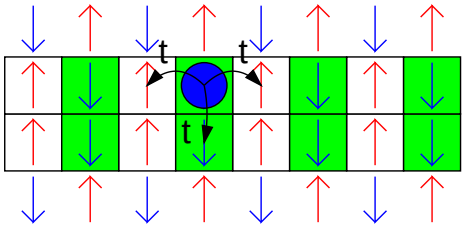

FIG. 9: We assume a single hole can move on the stripe and cannot leave the stripe. The surrounding antiferromagnet leads to staggered boundary conditions.

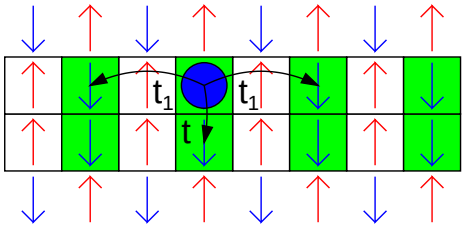

FIG. 10: For a one dimensional ladder with strong staggered potentials on the boundaries, a single hole effectively moves in steps of two.

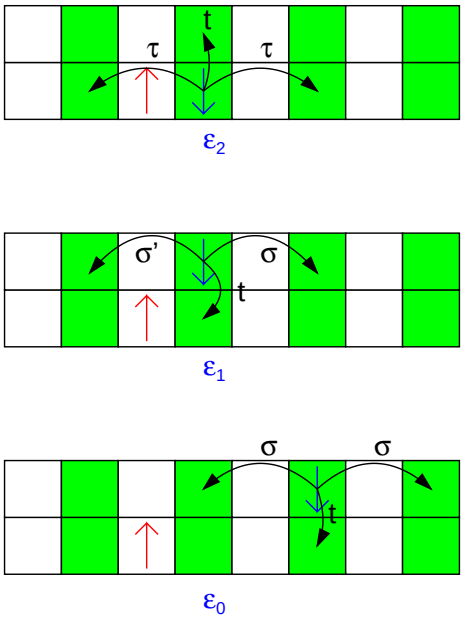

FIG. 11: Different possible configurations of two spins on a staggered two leg ladder.

the presence of the direct hopping term t allowed within the topological domain wall. This is in contrast to one dimensional effective theories that assume that the hole effectively becomes a holon on a stripe (see for instance Tchernyshyov and Pryadko[12]). Our hole is not a holon in the sense that it will remember if it was injected for a spin up or a spin down electron: they move on diffent sublattices.

We see that we can consider a single hole on a stripe as a quasiparticle, just as a single electron on an empty lattice. They can both be characterized by (different) values for ϵ_0 and σ. The main difference between a hole on a full ladder and an electron on an empty ladder is that the hole moves more slowly, because it can only move through double occupied intermediate states, which costs a lot of energy. Therefore, σ is small for a hole, while it is large for an electron on an empty lattice. Our main conclusion is that a single hole and a single electron are effectively identical.

IX. TWO ELECTRONS ON AN EMPTY STAGGERED LADDER

The equivalence between holes and electrons is no longer true for more than one particle. We will show that the low energy properties for two electrons are different from those of two holes. We first consider the problem of two electrons with opposite spin on an empty ladder. Various possible geometries are sketched in Fig. (11). Because only the relative distance is important, we keep the position of the up spin fixed.

The two electrons can be on the same or opposite legs. Six amplitudes: $\epsilon_0, \epsilon_1, \epsilon_2, \sigma, \sigma'$ and τ, defined in Fig. (11), are of relevance. We notice that the hopping amplitude for the electrons when they are far apart (σ) is much larger than the hopping amplitude when they are next to each other (τ). If they are far apart, they do not notice each other. Two electrons have less kinetic freedom if they are next to each other. In order to move passed each other, they have to go through a doubly occupied state.

In the $U \gg J$ limit, lowest order perturbation theory yields

$$\begin{aligned} \epsilon_1 = \epsilon_0 &= -2J - 4\frac{t^2}{2J}, \\ \epsilon_2 &= -2J - 2(\frac{t^2}{2J} + \frac{t^2}{2J+U}), \\ \sigma &= \frac{t^2}{2J}, \\ \tau &= \frac{t^2}{U+2J}. \end{aligned} \tag{15}$$

(16)

The lowest Hubbard sector contains both single electrons and pairs of electrons. However, we have seen that single electrons have a larger kinetic energy than pairs.

Therefore, the ground state consists of electrons that are as far apart as possible. Fig. (12) shows a schematic picture for the density of states. Only at the higher energies of the lowest Hubbard band do we find pairs. The pairs have a small bandwidth because of the small hopping amplitude. Once again we find various sectors as shown in Fig. (12).

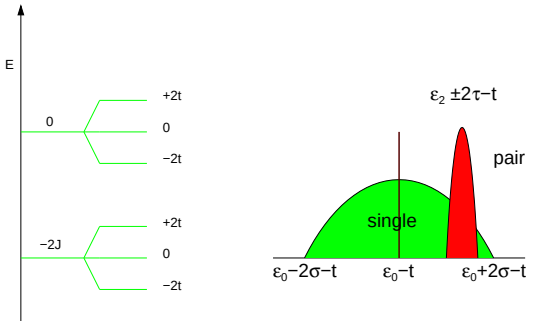

FIG. 12: Hubbard sectors for two spins on an empty ladder. The lowest Hubbard sector contains both single electrons and pairs of electrons. However, the groundstate consists of single electrons. Pairs are only formed at a higher energy in the lowest Hubbard sector.

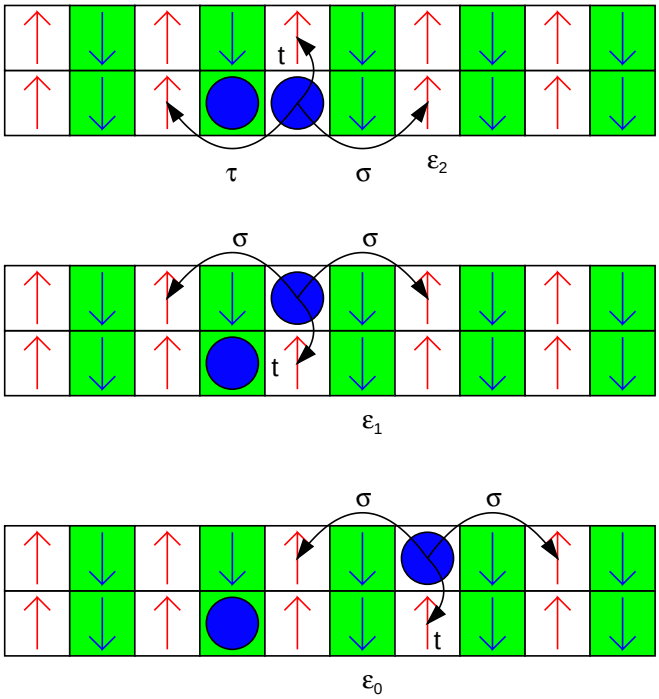

FIG. 13: Different configurations of two holes on a stripe with the relevant on site energies and hopping amplitudes.

X. TWO HOLES IN A FULL STAGGERED LADDER

To see the difference between electrons and holes, we now look at two holes in a filled ladder. When far apart, two holes (quasiparticles) do not notice each other. Just as for two electrons on an empty lattice, there are two states in which they strongly influence each other. The main question we wish to address is whether two holes come together and form a real-space pair, or if they tend to be as far apart as possible.

If the two holes are far apart, they will move independently with an amplitude $\sigma = \frac{t^2}{U+2J}$ (see Fig. (13)).

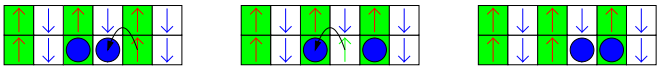

FIG. 14: Two holes can move together without creating an intermediate double occupied state. Therefore, holes want to form real-space pairs. A hole pair can move if a single electron makes two hops.

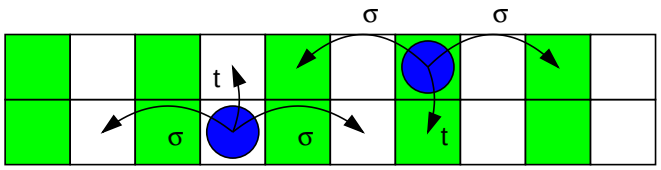

FIG. 15: We can neglect the spins on the ladder because they cannot change. This is caused by the boundary conditions.

However, this is different if they are sitting next to each other. In this case no double occupied state is needed. Therefore the hopping amplitude $\tau = \frac{t^2}{2J}$, thus $\tau \gg \sigma$.

If the two holes are on the same leg, sitting next to each other (see Fig. (14)), than the two holes can move together with a much larger amplitude than if they move alone.

In the left subfigure, a spin up electron moves left. The intermediate state in the middle figure has a higher energy of the order of J. From this position, the electron with spin up can move back to the starting position, or it can move on to end up as shown in the right figure. Once it is there, the hole-pair has effectively moved one site to the right. This figure only illustrates one possible hopping sequence, there are also other possible ways of hopping. For discussions of pairing one should be careful with fermionic minus signs sparked by the interchange of identical spins once a pair is made to go around[11,40]. For the movement of a single hole, there is an intermediate state with an energy of U. However, if the two holes are next to each other then the intermediate state will not have a doubly occupied site, so therefore this energy is only of the order of $4J$. Therefore, σ' is much large than σ. This leads to the formation of pairs on the stripe.

For large U and J, employing the same convention as before, we find in perturbation theory,

$$\begin{aligned} \epsilon_0 &= -(N-2)J - 4\frac{t^2}{2J} - (2N-8)\frac{t^2}{U+2J} \\ \epsilon_1 &= -(N-2)J - 4\frac{t^2}{2J} - (2N-8)\frac{t^2}{U+2J} \\ \epsilon_2 &= -(N-2)J - 2\frac{t^2}{2J} - (2N-6)\frac{t^2}{U+2J}, \end{aligned} \tag{17}$$

with $N = 2L$ the total number of sites on the two leg ladder.

The motion of the pairs on a ladder and the motion of single holes is coupled: both are present in the lowest Hubbard sector. If they form disjoint Hilbert spaces, we

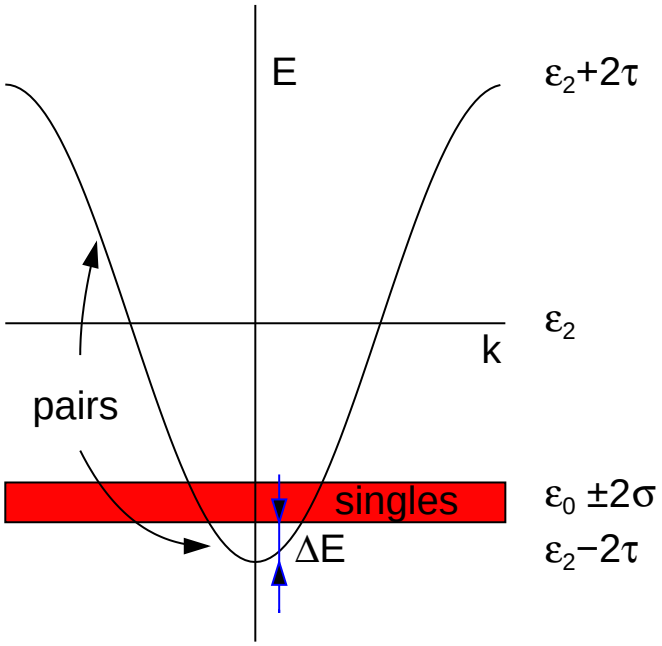

FIG. 16: Theoretical dispersion relation for two holes in a bond-centered stripe.The groundstate consists of pairs.

will find $E = \epsilon_2 - 2\tau \cos k$ for the real space pair. For two single holes, $E = \epsilon_0 - 2\sigma \cos k$, within perturbation theory. Because σ is very small, the spectrum for single hole states does not exhibit much dispersion. Taking the energy values from Eq. (18), the dispersion for two holes on a stripe with staggered potentials is suspected to look like that shown in Fig. (16).

The big difference between holes and electrons is that for two electrons the separated electrons have a large bandwidth and the pairs of electrons are a high energy state with a small dispersion. For holes this is reversed: the pairs have the largest bandwidth, while the separated electrons form a low energy excitation (string states) with a small dispersion.

The lowest state for the pair cosine band is located at $\epsilon_2 - 2\tau$ and the lowest state for the separated holes is located at $\epsilon_0 - 2\sigma$. In perturbation theory, both energies amount to

$$-(N-2)J - 4\frac{y^2}{2J} - (2N-8)\frac{t^2}{U+2J}. \qquad (18)$$

However, here we assumed the pairs and separated holes to be independent. But where they overlap in energy, which in this case is the bottom of the band, the wavefunctions will hybridize.

If we think of a hybridization of up and down sites along the rungs, then no possible interchange can be performed between the holes leading to fermionic minus signs that elevate, rather than depress, the pairing energy[11].

XI. LANCZOS CALCULATIONS

Lowest order perturbation theory for two holes on a staggered ladder leads to the dispersion shown in Fig. (15). The ground state properties cannot be easily determined because of the overlap between separate hole and pair states. To test this situation numerically, we have performed standard Lanczos calculations for the Hubbard model endowed with staggered boundary conditions on a twelve site single chain with staggered boundary conditions. Solving this problem for large two leg ladders is inhibited by the large Hilbert space. The maximum size which we are able to examine numerically is a 6×2 system for which there are $\approx 650,000$ states. Such a system is too small to observe single hole states and pairs accurately. Because of the strong bonding combination between the upper and lower leg of the ladder, the reduction to a one dimensional line is physically justified. The results of the Lanczos calculation show that the ground state has the largest amplitude for pair states with only a small admixture of single hole states. Immediately above the ground state, the excited states are predominantly single hole states. There is a finite energy gap separating the ground state and these excited states. Because of the small lattice size, we cannot determine the value of the energy gap ΔE.

Another approach is to assume that $\epsilon_0, \epsilon_2, \sigma$, and τ are adjustable parameters. In that case, we can perform a simplified calculation on a 20×2 ladder having twenty spin up, and twenty spin down sites. In the aftermath, this leads to a 400×400 matrix that can be easily diagonalized. Using this model it is relatively easy to choose the effective parameters such that the cosine band for the pairs has a lower energy than the states where we have single holes far apart. Our numerical results for the Lanczos method suggest that the gap ΔE separating pair states and single particle states is sufficiently large for the groundstate to consist mostly of pair states.

Nontheless, as the gap separating the single hole and pair states is small, the pairing physics is, a priori, susceptible to the addition of longer range interactions and hopping interactions. Such effects could easily tip the balance between the single hole and pair states (or enhance pairing tendencies).

XII. DMRG - PUTTING ALL OF THE PIECES TOGETHER

We found that if we assume that somehow the antiferromagnet has a ferromagnetic domain wall, holes will automatically localize on this topological line. Furthermore we looked at the movement of a single hole on this staggered ladder and found that it behaves as a single quasiparticle that moves along the ladder in steps of two. Two electrons on an empty lattice try to be as far apart as possible. Two holes on an otherwise halffilled ladder, however, form a bound pair. Fusing all of these findings

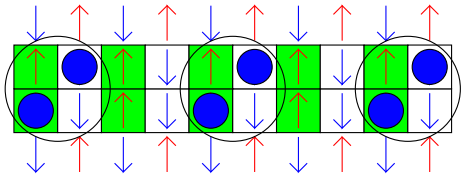

FIG. 17: If we have a quarter-filled stripe, we get the above picture for a stripe.

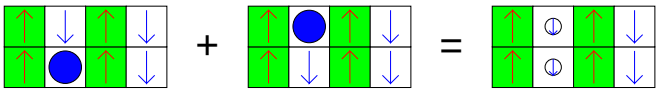

FIG. 18: The hole has equal amplitude to be on the upper or lower leg of the ladder. Therefore, the groundstate is a linear superposition of a hole and a spin down.

together, we obtain the stripes as seen by the DMRG calculations of White and Scalapino[8]. The arguments that we employed throughout were very pedestrian and general. Throughout we invoked the sublattice parity principle and the related staggering potentials. Our findings are further supported by numerical calculations on the t-J model. We give a very simple physical interpretation for the stripes found by DMRG.

A hole is on the stripe will delocalize by the hybridization of the upper and lower leg. If we place a hole on the upper leg, the hole will almost immediately jump to the lower leg and vice verse. In numerical calculations, we will therefore find the linear superposition of a hole and the electron depicted in Fig. (18).

White and Scalapino employed the DMRG technique on the t-J model[8]. Fig. (19) shows one of their well known results. We see that the bond centered stripes are very narrow. They look like a ferromagnetic seam in an antiferromagnet. The same result can be obtained in mean-field theory[41] as shown in Fig. (20).

The DMRG calculations of White and Scalapino vividly show how spin and charge nestle. White and

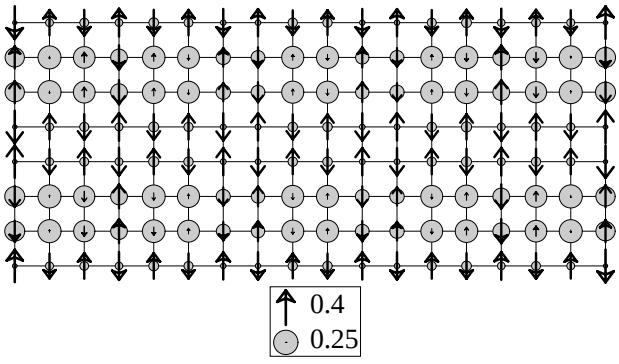

FIG. 19: The DMRG calculation of the t-J model by White and Scalapino[8]. This and similar calculations typically employ open or cylindrical boundary conditions.

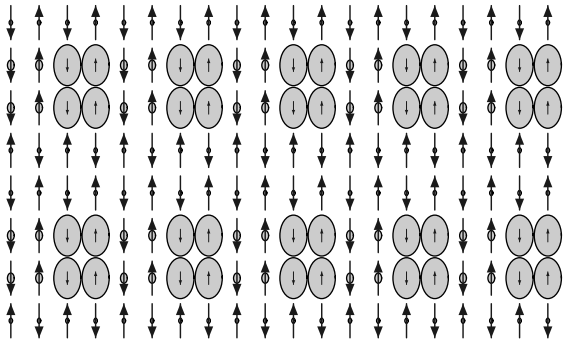

FIG. 20: Mean-field solution of the repulsive Hubbard model with U=8t. This calculation uses open boundary conditions.

Scalapino place much emphasis on the fact that again the holes are on next-nearest neighbor sites. On the opposite diagonal, the spins (which are on the same sublattice) have a very strong antiferromagnetic bonding. In effect, the bound pair is creating a flip in the antiferromagnetic lattice. This might also explain why in the exact calculations and the Monte-Carlo results the binding energy would decrease as a function of the lattice size. Basically, the hole-pair is creating an antiphase boundary, whose energy is increasing as a function of lattice size. That this is indeed a good representation of stripes follows from DMRG calculations by White and Scalapino. The reader is urged to focus on the central part of their picture- the spin and charge texture towards the boundaries are more contorted by the open boundary conditions employed. We will assume that Fig. (20) is a useful real-space representation of quarter-filled stripes. We claim that the reason that the mean-field[41] and the DMRG calculation are so similar has to do with the fact that the antiferromagnet is very strongly ordered. The stripes are so narrow because of *dynamical confinement*.

XIII. LONGER RANGE KINETIC AND COULOMB TERMS

Let us recapitulate the assumptions that we have invoked, so far, in our analysis:

(i) We assumed, self consistently, the existence of an antiphase domain wall having the geometry of a two leg ladder. Sublattice parity (Z_2) order was assumed to prevail throughout the entire system.

(ii) Albeit the relatively minute energy difference by which the lowest lying pair states were found to be favored over single hole states, we assumed that the stripe was composed entirely of pairs.

It should be noted (especially in the context of assumption (ii)), that the small energy differences we found separating various contending states (as well as those separating, say, bond centered stripes from site centered stripes) are very susceptible to additional terms in the Hamilto-

nian.

The Hubbard model or its t-J truncuation is only a model. There are myriad very important effects that it does not include which could easily shift the balance between various nearly degenerate contending states.

Coulomb effects (which are much greater importance here than elsewhere given the poor screening in these materials) enhance and stabilize stripe order: a uniform charge density order is strictly forbidden by the divergent Coulomb penalty that it will incur. This point has been emphasized by Emery, Kivelson, and coworkers[4],[42]. Fourier transforming the Hamiltonian and looking for the minimizing waveumbers, we are able to see how the charge density modulations will evolve and lead to stripe order[43] once lattice effects are taken into account.

Even if the stripe correlations found by the DMRG calculations of White and Scalapino on the pure t-J model are found to be due to open boundary condition effects, when long range Coulomb interactions are introduced, charge stripe order will be further stabilized. Given the natural coupling between spin and charge[44], this will further enhance the sublattice parity flips across the stripe that we assumed from the outset (assumption (i)).

Less emphasized are the role of higher order kinetic terms. These can easily tip the balance: a next nearest neighbor hopping increases pairing significantly. Within the pure t-J model (with a vanishing direct diagonal hopping amplitude $t' = 0$) pairing correlations are infinitesimal and are further frustrated by the π phase shift across the domain wall. Numerically, t' which allows holes to move on the same sublattice enhances pairing dramatically. Furthermore, numerically, a negative t' is seen to favor stripe formation[45].

XIV. CONCLUSION

We examined the consequences of hole motion in a strongly ordered antiferromagnet. We show that holes move to antiferromagnetic domain walls and effectively form two-leg ladders. This *dynamical confinement* of holes onto the stripe is caused by the sublattice structure of the antiferromagnet and the increase in kinetic energy on a domain wall. The effective two-leg ladders still feel the influence of the surrounding antiferromagnet in terms of a staggered boundary potential. As shown by Krotov, Lee, and Balatsky[38], this increases the tendency to superconductivity. The reason for this is that holes on the stripe form real-space pairs. Our results naturally lead to a theoretical description of the numerical results of White and Scalapino. Therefore, our starting assumption- the sublattice parity principle- and the neglect of string states that it entails might have some validity. Our article furnishes yet another example of a kinetic theory[11]- string states and magnetic (potential) effects of the like are not the immediate driving force for stripe formation and hole dynamics within our scheme.

In a upcoming paper we will show that these real-space pairs can be mapped to an effective one-dimensional XXZ model in a transverse field. This will allow us to discuss the filling fractions of stripes.

Appendix A: The sublattice parity principle

The sublattice parity principle amounts to the assumption that a hole in an antiferromagnet is free and can move to all of its *next* nearest but not to its direct neighbors. This principle is based on and follows from the sublattice structure of antiferromagnetic order. We will provide phenomenological proof for this assumption by examining the dispersion relations obtained by very detailed numerical works.

1. Spin flips

It is well known that the Hubbard model for a half-filled system in the large U limit leads to an effective Heisenberg model,

$$H_{\rm Heisenberg} = \sum_{\langle ij \rangle} \frac{J_\perp}{2}(S_i^+ S_j^- + S_i^- S_j^+) + J_z S_i^z S_j^z, \quad \text{(A1)}$$

with $J_\perp = J_z = J$.

The last (Ising) term of the Heisenberg Hamiltonian wants to make the spins on neighboring lattice sites point in opposite directions. If only this term is present, the groundstate will be a perfect Ising antiferromagnet with long-range (Néel) order: the lattice can be subdivided in an up sublattice and a down sublattice. However, the first (XY) term in the Hamiltonian can undo this order by flipping two neighboring, opposite spins. In principle this term can completely destroy the long range order and indeed it does so in one dimension. In dimensions $d \geq 3$ clear sublattice order prevails. A large amount of effort in numerical calculations and the very important analysis of the non-linear sigma model by Chakravarty, Halperin and Nelson[46] have shown that the ground-state of the two-dimensional Heisenberg model (and thus of the undoped Hubbard model) is a long range antiferromagnet for which there exists a two-sublattice structure. The groundstate of the antiferromagnet is not exactly given by the classical Néel state which one would expect

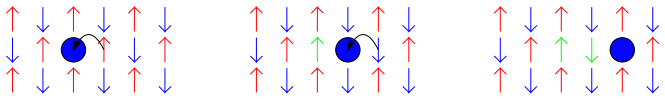

FIG. 21: If a single hole in an antiferromagnet moves by nearest neighbor hopping of surrounding spins, it cannot move without creating a string of flipped spins. For small values of $J_\perp$, there are no spin flips that can destroy this string. This leads to a linearly increasing confining potential and the eigenfunctions are Airy wave functions. Because of this string, a single hole cannot easily propagate through an antiferromagnet by nearest neighbor hops.

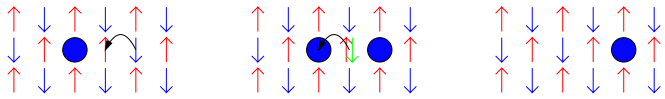

FIG. 22: A single hole can still move through an antiferromagnet without generating string states by hopping in steps of two. This way it stays on the same sublattice. For this it has to go through an intermediate state with a double occupied site. This intermediate state costs an energy U. This leads to movement of the hole on the same sublattice with an amplitude $\propto t^2/U$.

from the Ising model. The spin-flip term leads to a finite density of flipped spins (approximately 20%) which give rise to a lowering of the magnetization. It also leads to spin-waves. These spin-waves destroy the long-range antiferromagnetic order at any finite temperature. However, one can define a correlation length and on distances smaller than this length, we can still speak about local antiferromagnetic order. For $T > 0$, we have local order with a correlation length that decreases with increasing temperature. Therefore, thinking in terms of an Ising model is not completely incorrect as long as one keeps in mind that there is a finite density of flipped spins in the lattice. In the remainder of this article we will neglect these spin flips.

A moment's reflection reveals that $[H, S_z^{tot}] = 0$ for the Hubbard model (a property inherited to its descendants), and net magnetization is strictly preserved. Consequently, if Néel order prevails also when a single hole is introduced, hole motion is rigorosly restricted to one sublattice: if a hole could indeed hop to its neighboring site on the opposite sublattice, the magnetic quantum number $(S_z/\hbar)$ would remain unaltered. On the other hand the two low energy "vacuum" states corresponding to the injection of a hole on the two different sublattices have magnetic quantum numbers $(S_z/\hbar)$ differing by ± 1. These states obviously cannot be connected by any of the magnetization conserving processes of H. Myriad analytical treatments of the t-J and Hubbard models were aware of this selection rule and have computed transition matrix elements for a single hole between sites of the same sublattice. For one example amongst many see[47].

A well known argument leads to the conclusion that a single hole cannot propagate freely in an antiferromagnet. As shown in Fig. (21), whenever a non backtracking single hole moves from one sublattice to the other, it creates a string of flipped spins in its wake. This leads to a linear confining potential that strongly inhibits hole motion between different sublattices.

This, however, is not the only process that can take place. Fig. (22) shows that it is also possible for a hole to move two steps without creating a confining string potential. This is a second order process in perturbation theory. First we create a second hole two sites away from the first hole. We do this by moving that electron one site closer, next to the first hole. This gives rise to a double occupied intermediate state with a high energy U. Then, we let the same electron move again, now removing the first hole. The amplitude for the total process is given by $\sigma = \frac{t^2}{U}$, much smaller than t, the first order hopping amplitude. However, the final state has exactly the same energy as the starting state. There are eight sites to which a single hole can hop in this fashion. Note that throughout the entire process, the magnetic quantum number in Fig. (22) is preserved, e.g. $S_z^{tot} = \hbar/2$ if perfect Néel order prevails everywhere around the fragment displayed in the figure for a lattice with an even number of sites. Within the t-J and $t - J_z$ approximations to the Hubbard model, same sublattice hops are more masked. In the t-J model, only a third order process links a hole to one of its next nearest neighbors on the same sublattice. Albeit holding for models derived from the Hubbard model on bipartite lattices, in many instances the sublattice parity principle becomes much more alive and transparent within the original Hubbard model itself.

2. Numerical dispersions

Simulations of the Hubbard and Heisenberg model with a single hole have found a discrete number of sharp peaks in the spectrum which could be identified with string-states. The longer the string, the higher the energy of the peak. Because there is a gap between the first and second peak, we can confine our attention to the lowest peak. This peak has a finite quasi-particle weight. The dispersion of this peak as a function of k, tells us about the effective movement of a hole through an antiferromagnet. A numerical result from Louis *et. al.*[25] for this dispersion relation in the Hubbard model is shown in Fig. (23).

The central result of numerous investigations is that they all found that a sharp quasiparticle peak appears at the bottom of a broad continuum of the hole spectrum. These quasiparticle poles form a coherent hole band with a width of order of $2J$ over a wide range of J/t, and the coherent propagation is made possible by "healing" a string of flipped spins by quantum fluctuations.

One can easily Fourier transform the numerical low energy hole dispersion relation $\epsilon(\vec{k})$ to unveil the important real space quasiparticle motions and their respective am-

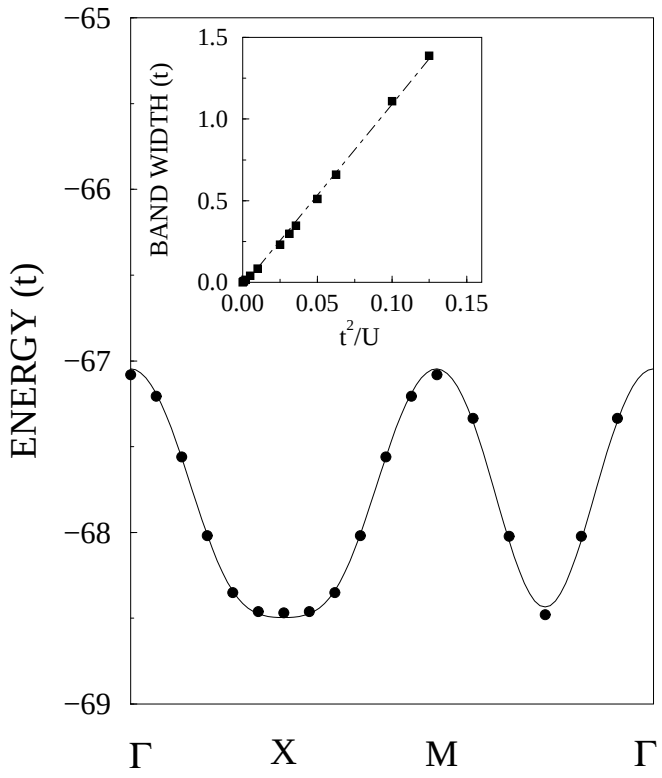

FIG. 23: Quasiparticle band structure for a single hole on 12×12 clusters of the square lattice with periodic boundary conditions and $U = 8t$. The solid line corresponds to the fitted dispersion relation (see text). The inset shows the bandwidth as a function of t^2/U for $U \geq 8t$; the fitted straight line is $-0.022t + 11.11t^2/U$. From Louis, Guinea, López Sancho and Vergés[25].

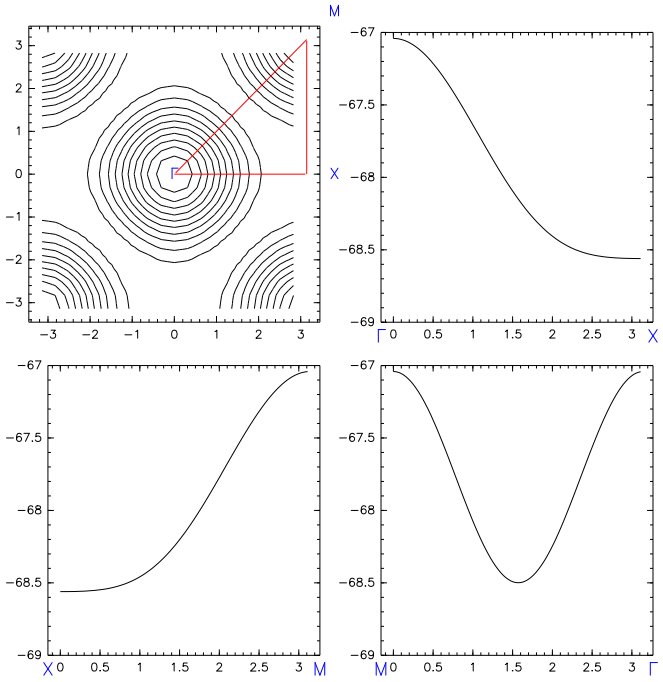

FIG. 24: Dispersion relation for a single hole in an antiferromagnet according to the simple view that the hole is a quasi-particle that moves on one sublattice by hopping in steps of two (equation A2). Here we employ $\epsilon_0 = -68.15t$, $t_2 = -1.52\frac{t^2}{U}$ and $t_0 = -0.70\frac{t^2}{U}$ with $U = 8t$.

plitudes. If we make the simplifying assumption that the hole is the quasiparticle then we find that essentially all of the low energy weight is distributed amongst the next nearest neighbor motions linking the hole to its sublattice. This is a consistent logical outcome of a strong local Néel order fused with the fact that the magnetic moment is a conserved quantum number. That the nearest states on the same sublattice (and those further away) have the highest weight could hardly be surprising. Hopping amplitudes to sites which are further and further away on the same sublattice drops significantly with distance[25].

Stated alternatively, if on the two dimensional lattice, the hopping amplitude to any of the four colinear sites (twice (up, down, right or left)) is t_0 and if motion to any of the four diagonal sites has amplitude t_2) then the dispersion relation will read

$$\epsilon_k = \epsilon_0 - 4t_2 \cos k_x \cos k_y - 2t_0(\cos 2k_x + \cos 2k_y). \quad \text{(A2)}$$

From lowest order perturbation theory[47], we immediately expect $t_2 = 2t_0 = -\mathcal{O}(\frac{t^2}{U})$ where the relative factor of two originates from the two paths by which we may reach diagonal sites by two consecutive hops as comparde to the single two step route to longintudinal next nearest neighbors. As illustrated in Fig. (24), renormalized hopping amplitudes of the same order of magnitude $\mathcal{O}(\frac{t^2}{U})$ reproduce the detailed and tedious numerical fits of Fig. (23) remarkably well. More generally, if one Fourier transforms the elaborate data encoded in Fig. (23) we find that the bulk of the Fourier weight corresponds to next to nearest neighbor motions with hopping amplitudes of the same order as anticipated from lowest order perturbation theory[25].

In accordance with expectations from perturbation theory, it is indeed found numerically that diagonal (*nodal*) hopping is almost twice as large in amplitude as compared to longitudinal hopping (a property which might easily transcend to larger length scales by virtue of many of the small length scales in these materials) with both amplitudes of order $\mathcal{O}(\frac{t^2}{U})$. In Fig. (24), we show the theoretical dispersion curves coming from equation (A2) for $t_0 = -0.70\frac{t^2}{U}$ and $t_2 = -1.52\frac{t^2}{U}$ and $\epsilon_0 = -68.15t$. These curves capture all the essential features of the numerical dispersion curve shown in Fig. (23).

It is obvious that the Brillouin zone has doubled as a result of the fact that the hole is moving in steps of two through the lattice.

The very good fit obtained to the dispersion curve of a single hole in an antiferromagnet by introducing the

three parameters (ϵ_0, t_0 and t_2) suggests that the complicated problem of a single hole in an antiferromagnet can be reduced to a single particle problem. This is a major simplification. If we really can neglect spin-flips and string-states, the single hole problem has been reduced to a single-particle problem. The spins have become static and their only function is to create a checkerboard like sublattice structure that keeps the hole moving on only one sublattice by forcing it to move in steps of two. Large J means in principle both large J_z and $J_\perp$. A large $J_\perp$ leads to spin-flips being relatively important and this will restore the string-states. Increasing the value of J, and thus of $J_\perp$, leads to spin-flips which will restore a string to the normal antiferromagnet. However, the relevant region of the Hubbard model and the t-J model is the region of small values of J.

Stated in more general terms, the constraint on the motion of the holes (equivalent to the assumption of Néel order) may be regarded as a low energy selection rule on the matrix elements of the effective Hamiltonian. The total z component of spin (sublattice parity order) is a conserved quantum number and transitions between different sublattice states are banned. Whenever Néel order is strong, the states are effectively separated into two disjoint Hilbert spaces each for a different sublattice parity (magnetic S_z) quantum number. As we demonstrate in the main text, stripe order may be interpreted as an immediate consequence of sublattice parity quantum numbers.

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