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Hole on a stripe in a spinless fermion model

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Abstract. – In the spinless fermion model on a square lattice with infinite nearest-neighbor repulsion, holes doped into the half-filled ordered state form stripes which, at low doping, are stable against phase separation into an ordered state and a hole-rich metal. Here we consider transport of additional holes along these stripes. The motion of a single hole on a stripe is mapped to a one-dimensional problem, a variational wave function is constructed and the energy spectrum is calculated and compared to energies obtained by exact diagonalization.

Introduction. – A spinless square lattice fermion model with nearest-neighbor repulsion, we suggest, may be a fruitful and comparatively tractable analog of the Hubbard model that retains many of its properties. In particular, in the limit of infinite repulsion, near half-filling, the equilibrium state appears to be an array of charged, antiphase domain wall stripes that are stabilized by kinetic energy [1, 2]. This is reminiscent of a state of charged stripes that has been observed in cuprates [3] and has been discussed in the spinfull Hubbard and t-J models [4]. Stripes in the spinless fermion model have been studied by exact diagonalization (ED) in ref. [2]. Here we are interested in finding to what extent a hole, moving along a stripe, is decoupled from the state of the stripe, and whether or not the hole tends to bind to a "kink" on the stripe. To this end we extend an exact mapping of a stripe to one dimension, introduced in refs. [1, 2]. Using this mapping, we construct a variational wave function and calculate the energy spectrum.

We do not know of an existing experimental system that realizes our model, but recent progress in the manipulation of ultracold bosonic atoms on an optical lattice [5], and in cooling fermionic atoms below degeneracy temperature [6], leads us to expect that such a model may be realized experimentally in the near future. A corresponding hard-core boson model with large nearest-neighbor repulsion can be realized, on a triangular lattice, in adsorption of ^{4}He to graphite sheets [7]. The phase diagram of a boson model with finite nearest-neighbor and next-nearest-neighbor repulsion was studied in ref. [8].

Model. – We consider spinless fermions on a square lattice with Hamiltonian

$$\mathcal{H} = -t \sum_{\langle ij \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i \right) + V \sum_{\langle ij \rangle} c_i^\dagger c_i c_j^\dagger c_j, \tag{1}$$

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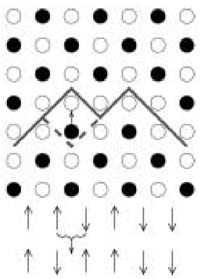
Fig. 1

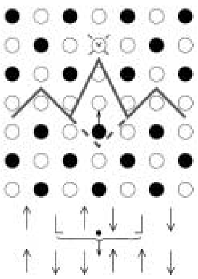
Fig. 2

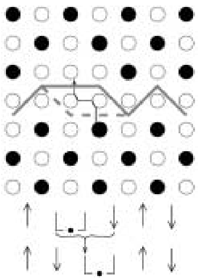
Fig. 3

Fig. 1 – Particle hops (stripe fluctuations) in an undoped stripe are equivalent to spin exchange.

Fig. 2 – Hole stranding: stripe fluctuation across the hole can leave the hole away from the stripe, with no possible allowed hops. We ignore these moves in our variational model.

Fig. 3 – Three successive moves that shift the hole by one position to the right. The sequence shown here is a *main path* sequence that can occur regardless of the configuration of the stripe.

where $c_i^\dagger$ and c_i are creation and annihilation operators at site i, respectively, and $\langle ij\rangle$ means nearest neighbors. In this paper, we consider only the limit of zero temperature and $V/|t| = \infty$, so that neighboring fermions are forbidden, and $t \equiv 1$ is the only energy scale. The maximum allowed filling fraction is $n = 1/2$, where there are two possible "checkerboard" states [9]. To make a well-defined situation, we assume a finite system with periodic boundary conditions having dimensions $L_x \times L_y$, where L_x is even and L_y is odd. This forces an odd number of domain walls (which must be stripes) running in the x-direction. These domain walls are composed of 1/2 of a hole per column and we call them *stripes*. This model has been studied by ED for spinless fermions and hard-core bosons, and the stripes were shown to be stable against phase separation, for fermions [1, 2]. When the number of particles is $L_x(L_y-1)/2$, only one stripe is allowed. If we remove a few more particles (less than L_x), it is energetically favorable for the holes to attach to the stripe, since holes off the stripe can only form confined droplets [9]. From here on, we reserve the term "hole" for additional holes beyond those needed to create a stripe. In the case of a single undoped stripe, the boson and fermion models possess the same energy spectrum [2].

On an undoped stripe, hops of particles are equivalent to stripe fluctuations (see fig. 1). If we define the stripe height $y(x)$ to be the mean of the y coordinates of the first particles above and below the stripe, in column x, we can map the up and down steps of the stripe height to "spins" in one dimension by defining $s(x) = \frac{1}{2}[y(x) - y(x-1)]$, taking values $\pm 1/2$. The corresponding Hamiltonian is the one-dimensional spin-(1/2) XY Hamiltonian

$$\mathcal{H}_{ex} = -\sum_i \mathcal{H}_{ex}^i, \quad \text{where } \mathcal{H}_{ex}^i = S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+, \tag{2}$$

where S_i^+, S_i^- are spin-raising and -lowering operators. This model can be solved by the Jordan-Wigner transformation, in which we replace each up-spin by a spinless fermion, and each down-spin by an empty space. The Hamiltonian is replaced by a non-interacting hopping Hamiltonian for the fermions. Thus, the ground state of a horizontal, undoped stripe is equivalent to that of a (one-dimensional) half-filled sea of free (spinless) fermions with dispersion $\epsilon(k) = -2\cos k$. From this, the ground-state energy, for large L_x, is $\epsilon_0^{(L_x)} = -2L_x/\pi$. This implies the chemical potential of the stripe is $\mu_{\text{stripe}} = -4/\pi$, since half of a particle is removed per unit length of a stripe. In a more general case, we may force a stripe with some overall tilt by replacing our rectangular boundary conditions with $(L_x, b) \times (0, L_y)$, for $L_x + b$ even. In that case the spin chain has total spin b, mapping to 1D fermions results in $N = (L_x + b)/2$ fermions and the ground-state energy is $\epsilon_0^{(L_x,N)} = -2L_x \sin(N\pi/L)/\pi$ [2, 10]. Note that a diagonal stripe ($b = L_x$) has zero energy, as there are no allowed hops.

One hole on a stripe. – If an additional hole is added to a stripe, the energy is lowered due to the hopping energy of the hole along the stripe. We define the ground-state energy difference $\Delta \equiv E_{\text{hole}} - E_{\text{stripe}}$, where E_{hole}, $E_{\text{stripe}} = \epsilon_0^{(L_x)}$ are ground-state energies of a stripe with a hole and an undoped stripe, respectively. For stability of a stripe array state, we must have $\Delta > \mu_{\text{stripe}}$; otherwise, doping would add holes to existing stripes, probably forming a phase-separated droplet. To obtain a variational bound for Δ, we will make (below) an approximation by using a subset of the Hilbert space.

Once a single hole is added to column x of the stripe, the stripe height difference in the two columns adjacent to the hole can take values of 0 or ± 2 rather than ± 1, *i.e.* $s(x), s(x+1) \in \{0, \pm 1\}$ (see, for example, figs. 2, 3). Thus, we get a pair of "spin-1" impurities on both sides of the hole, at positions x and $x+1$ on the spin chain. This looks like a Kondo model with two mobile impurities, that are bound together. Similar systems, with *t-J* Hamiltonian and mobile spin-(1/2) impurities in a spin-1 chain, have been the subject of theoretical study, as a model for the charge transfer insulator $Y_{2-x}Ca_xBaNiO_5$ [11]. However, our model is quite different from those, because the hopping matrix is quite elaborate, reflecting the allowed moves in the original stripe.

In order for our variational scheme to work, we need to separate the "hole degrees of freedom" from the "stripe degrees of freedom". To make this separation apparent, we find it more convenient to introduce a different, equivalent notation, in which the stripe and the hole are represented by a one-dimensional spin-(1/2) chain of length $L'_x \equiv L_x - 2$, with three additional "particles": a hole (represented by a dot), that marks the position of the hole in between two spins, and two "brackets" (right and left), each taking the place of a spin. If $s(x+1) = 1$ (-1), then the right bracket takes the places of the first down- (up-) spin to the right of the hole, and $s(x+1)$ is set to 1/2 $(-1/2)$. If $s(x+1) = 0$, the right bracket is placed in position $x+1$. Similarly for the left bracket and $s(x)$. Note that the total spin is preserved by this mapping. For example, if we use a double arrow to denote $s(x) = \pm 1$,

$$\begin{array}{cccccccccccccccccccc}
\downarrow & \uparrow & \downarrow & \downarrow & \downarrow & \Downarrow & \Uparrow & \downarrow & \downarrow & \uparrow & \Longrightarrow & \downarrow & \lfloor\downarrow & \downarrow & \downarrow & \downarrow\cdot & \uparrow\rfloor & \downarrow & \uparrow \\
\downarrow & \uparrow & \downarrow & \downarrow & \downarrow & 0 & \Downarrow & \downarrow & \uparrow & \uparrow & \Longrightarrow & \downarrow & \uparrow & \downarrow & \downarrow & \downarrow\lfloor\cdot & \downarrow & \downarrow\rfloor & \uparrow \\
\uparrow & \downarrow & \uparrow & \uparrow & \uparrow & \Uparrow & \Uparrow & \uparrow & \uparrow & \downarrow & \Longrightarrow & \uparrow & \lfloor\uparrow & \uparrow & \uparrow & \uparrow\cdot & \uparrow & \uparrow & \uparrow\rfloor
\end{array} . \tag{3}$$

If stripe fluctuations occur in the vicinity of the hole, it might become *stranded*, *i.e.* isolated from the stripe, as in fig. 2. However, we observe that in the ED ground state of ref. [2], the probability for this to occur is negligible (about 0.03 for an untilted stripe and less than 0.01 for a tilted one). Thus, in the following discussion we suppress hops that lead to the stranded state. Under this assumption, the spin chain is free to fluctuate only outside the brackets. Each of the three additional "particles" can hop by one step freely, as long as all of the spins between the hole and each of the brackets are in the same direction, and as long as their order is preserved (*i.e.* they do not hop across each other). This mapping can be shown to be exact.

The Hamiltonian for the hole on the stripe in this model can now be broken up: $\mathcal{H}_{\text{hole}} = \mathcal{H}_h + \mathcal{H}_r + \mathcal{H}_l + \mathcal{H}'_{sp}$, where $\mathcal{H}_h$, $\mathcal{H}_r$, $\mathcal{H}_l$ are the hopping terms for the hole, right bracket and left bracket, respectively, and $\mathcal{H}'_{sp}$ is the spin exchange Hamiltonian acting only outside the brackets. The Hamiltonian $\mathcal{H}_{\text{hole}}$ acts on the Hilbert space of "allowed states", *i.e.*, all

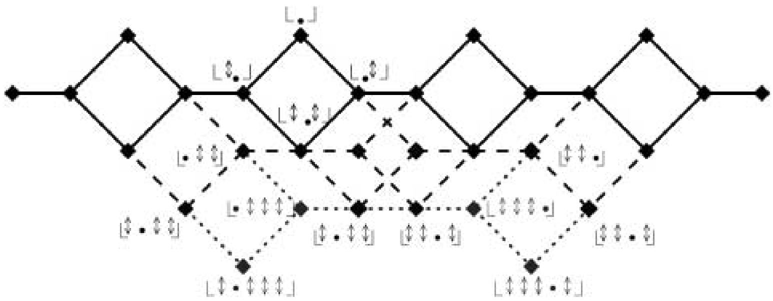

Fig. 4 – State space representation of hole motion for a particular background stripe/spin configuration. The $\updownarrow$ symbol represents an unspecified spin ($\uparrow$ or $\downarrow$). The solid lines represent the "main path", in which the hole motion is decoupled from its environment. The dashed and dotted lines represent the additional available hops when there is a run of two or three spins in the same direction, respectively. If we read this from left to right, a horizontal line represents one hop of the hole to the right, a downward (upward) diagonal line represents hopping of the right (left) bracket.

states in which the spins between each of the brackets and the hole are in the same direction. We denote the state of the hole and two brackets by $|x, l, r\rangle$, where the hole is between the spins at positions x and $x+1$, there are l spins (sites $[x-l+1, x]$) between the hole and left bracket, and r spins between the hole and the right bracket (sites $[x+1, x+r]$). For example, in the three examples in (3) above, if we number the spins starting from 1 at the left, the hole+bracket states are $|5,4,1\rangle$, $|5,0,2\rangle$, $|5,4,3\rangle$, respectively. Using this notation

$$\mathcal{H}_h = -\sum_{x,l,r} \delta_{r>0}\big(\mathcal{P}^{SS}_x + \delta_{l,0}\big(1-\mathcal{P}^{SS}_x\big)\big)|x,l,r\rangle\langle x+1, l+1, r-1| + \text{h.c.}, \tag{4a}$$

$$\mathcal{H}_r = -\sum_{x,l,r} \big(\mathcal{P}^{SS}_{x+r} + \delta_{r,0}\big(1-\mathcal{P}^{SS}_{x+r}\big)\big)|x,l,r+1\rangle\langle x,l,r| + \text{h.c.}, \tag{4b}$$

$$\mathcal{H}_l = -\sum_{x,l,r} \big(\mathcal{P}^{SS}_{x-l} + \delta_{l,0}\big(1-\mathcal{P}^{SS}_{x-l}\big)\big)|x,l+1,r\rangle\langle x,l,r| + \text{h.c.}, \tag{4c}$$

$$\mathcal{H}'_{sp} = -\sum_{xlr} |x,l,r\rangle\langle x,l,r|\bigg(\sum_i{}' \mathcal{H}^i_{ex}\bigg), \tag{4d}$$

where $\mathcal{P}^{SS}_x \equiv 2S^z_x S^z_{x+1} + 1/2$ is 1 if $S^z_x = S^z_{x+1}$ and zero otherwise, and $\sum'$ denotes a sum only on sites that are outside of the brackets ($i \notin [x-l, x+r]$). We have thus obtained that, using the mapping, the coupling between the hole and spin degrees of freedom seems to be limited to the interval between the brackets. Therefore, it is natural to construct a variational wave function by starting with a complete decoupling between the hole and the stripe, and project out the "illegal" states, in the spirit of the Gutzwiller projection.

Motion of a hole on a stripe. – In order to examine the motion of a hole on a stripe, we find it instructive to represent the various states of the stripe by a *state graph* [2], which is defined such that each node represents a state and each line represents an allowed hop between states. In order for the hole and brackets to shift by one position, in this model, three individual hops are required (see, *e.g.*, fig. 3). Generally, it is clear that the allowed hole and bracket moves depend on the background stripe configuration. The simplest possible motion is when each of the brackets does not stray more than one position away from the hole, thereby eliminating any dependence on the stripe. This motion can be represented in the state space by the solid lines in fig. 4, and we refer to it as the "*main path*". Depending on the local tilt in the stripe (runs of spins in the same direction), the available states are increased. In the extreme case, if the stripe is a 45° diagonal, then the hole and brackets can be treated as three non-interacting fermions and their energy is lower than in the untilted case. This implies that the hole prefers the stripe to be locally tilted around it. However, the spin chain loses energy by having a region where all of the spins are the same, since no spin exchange is possible there. We would expect the interplay between these two competing effects to result in a small tilted region ("kink") around the hole. This has indeed been inferred from ED of ref. [2], and is one of the phenomena that we look for in our solution for this model.

Examining the motion of a single hole on a stripe, we find that any sequence of moves that returns the system to its original configuration involves an even permutation, except for hole hopping around odd boundary conditions [12]. This implies that for even or infinite L_x, the boson and fermion spectra are identical.

Variational wave function. – In order to calculate the hole spectrum variationally, we introduce a projection operator $\mathcal{P}^{\alpha\beta}_{lr}(x)$ acting on states of a spin chain of length L'_x, to the sub-space where all of the l spins at sites $[x-l+1,x]$ are in direction α, and r spins at positions $[x+1,x+r]$ are in direction β ($\alpha,\beta\in\{\downarrow,\uparrow\}$). $\mathcal{P}^{\alpha\beta}_{lr}(x)$ annihilates states that are not in this subspace. We define an orthonormal basis set:

$$\chi^{\alpha\beta}_{lr}(x)=\frac{1}{\mathcal{N}^{\alpha\beta}_{lr}}|x,l,r\rangle\mathcal{P}^{\alpha\beta}_{lr}(x)|\Phi_F\rangle, \tag{5}$$

where $|\Phi_F\rangle$ is the ground state of an unrestricted spin-(1/2) ring of length L'_x; $\mathcal{N}^{\alpha\beta}_{lr}=\sqrt{\langle\mathcal{P}^{\alpha\beta}_{lr}\rangle_F}$ is a normalization factor, where $\langle\mathcal{P}^{\alpha\beta}_{lr}\rangle_F\equiv\langle\Phi_F|\mathcal{P}^{\alpha\beta}_{lr}(x)|\Phi_F\rangle$ is independent of x.

Now we want to calculate $\langle\chi^{\alpha\beta}_{lr}(x)|\mathcal{H}_{\rm hole}|\chi^{\alpha'\beta'}_{l'r'}(x)\rangle$. The matrix elements for $\mathcal{H}_h$, $\mathcal{H}_r$, $\mathcal{H}_l$ are straightforward, but those of $\mathcal{H}'_{sp}$ are a little harder to calculate. Since $\mathcal{H}'_{sp}$ does not change the hole+brackets state $|x,l,r\rangle$, we only need matrix elements between pairs of states with the same x, l, r, *i.e.* $\langle\chi^{\alpha\beta}_{lr}(x)|\mathcal{H}'_{sp}|\chi^{\alpha'\beta'}_{lr}(x)\rangle$. These can be calculated using the fact that $\mathcal{H}'_{sp}$ commutes with $\mathcal{P}^{\alpha\beta}_{lr}(x)$:

$$\begin{aligned}\left\langle\chi^{\alpha\beta}_{lr}(x)\middle|\mathcal{H}'_{sp}\middle|\chi^{\alpha'\beta'}_{lr}(x)\right\rangle &= \frac{1}{\mathcal{N}^{\alpha\beta}_{lr}\mathcal{N}^{\alpha'\beta'}_{lr}}\left\langle\mathcal{P}^{\alpha\beta}_{lr}(x){\sum_i}'\mathcal{H}^i_{ex}\mathcal{P}^{\alpha'\beta'}_{lr}(x)\right\rangle_F\\ &= \frac{1}{\left\langle\mathcal{P}^{\alpha\beta}_{lr}\right\rangle_F}\tilde{\delta}^l_{\alpha,\alpha'}\tilde{\delta}^r_{\beta,\beta'}\left\langle\mathcal{P}^{\alpha\beta}_{lr}(0){\sum_i}'\mathcal{H}^i_{ex}\right\rangle_F\\ &= \tilde{\delta}^l_{\alpha,\alpha'}\tilde{\delta}^r_{\beta,\beta'}\left[\epsilon_0^{(L'_x)}-\frac{\left\langle\mathcal{P}^{\alpha\beta}_{lr}(0)\left(\mathcal{H}^{x-l}_{ex}+\mathcal{H}^x_{ex}+\mathcal{H}^{x+r}_{ex}\right)\right\rangle_F}{\left\langle\mathcal{P}^{\alpha\beta}_{lr}\right\rangle_F}\right],\end{aligned} \tag{6}$$

which is independent of x. We used i) $[\mathcal{H}^i_{ex},\mathcal{P}^{\alpha\beta}_{lr}(x)]=0$ for $i\notin[x-l,x+r]$ (modulo L'_x); ii) $\mathcal{P}^{\alpha\beta}_{lr}(x)\mathcal{H}^i_{ex}=0$ for $i\in(x-l,x)$ or $i\in(x,x+r)$. Note that when $l=0$, α is undefined, so in order to generalize the notations, we arbitrarily set $\alpha=\downarrow$ when $l=0$ ($\mathcal{P}^{\uparrow\beta}_{l=0,r}=0$), and similarly for r, β. We defined $\tilde{\delta}^l_{\alpha,\gamma}\equiv\delta_{\alpha,\gamma}$ if $l>0$ and $\tilde{\delta}^l_{\alpha,\gamma}=0$ otherwise. In order to calculate the energy spectrum using the variational wave function, we Fourier transform $\chi^{\alpha\beta}_{lr}(x)$ and find $\langle\chi^{\alpha\beta}_{lr}(k)|\mathcal{H}_{\rm hole}|\chi^{\alpha'\beta'}_{lr}(k)\rangle$ in a straightforward manner.

Results. – The results presented here were obtained for a subset of the variational basis set with $l+r\le 10$ for our calculations. If one does not take advantage of mirror symmetries

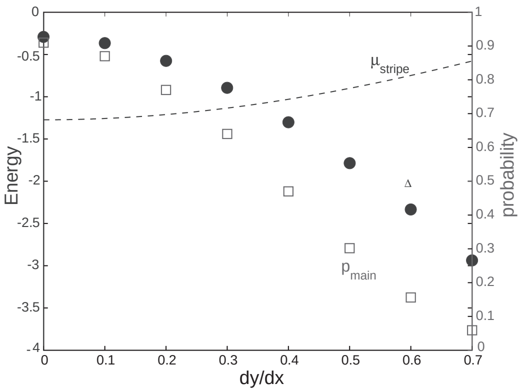

Fig. 5

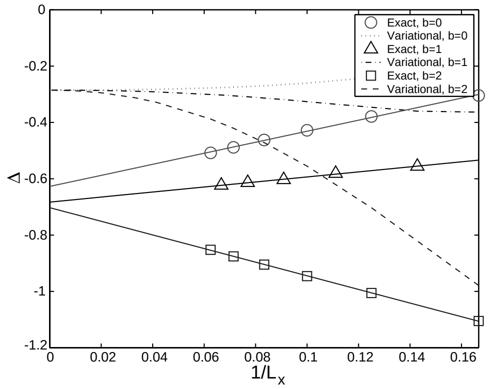

Fig. 6

Fig. 5 – Circles: ground-state energy difference $\Delta \equiv E_{\rm hole} - E_{\rm stripe}$ as a function of overall stripe tilt, for infinite L_x. The dashed line represents the chemical potential $\mu_{\rm stripe}$. ($\mu_{\rm stripe} < \Delta$ is required for stripe stability.) Squares: main path probability $P_{\rm main}$.

Fig. 6 – Energy difference Δ obtained in ED and variational calculations, for finite system sizes. Results are shown for horizontal stripes ($b = 0$), as well as tilted boundary conditions ($b = 1$, 2). The solid lines are linear interpolations of the ED data. Note that although Δ decreases as the tilt increases, $E_{\rm hole}$ generally increases with tilt.

between states, the Hamiltonian is a 221×221 matrix. We find the ground state and ground-state energy of this Hamiltonian as a function of L_x, b, and k. Increasing the variational basis set to up to $l + r \leq 13$ results in a relative change of less than 0.1% in Δ for the maximum overall tilt presented here, and less than 10^{-14} for zero tilt. In our calculation, we take into account the fermion statistics only by adding a phase to hole hops in (finite) odd boundary conditions. This is justified because these are the only moves that can induce an odd cyclic permutation of the particles [12].

Figure 5 shows the ground-state energy difference Δ, as a function of the overall stripe tilt. We obtain $\Delta = -0.29$ for an (infinite) untilted stripe. As the stripe tilt is increased, both the energy of the undoped stripe, $E_{\rm stripe}$, and $E_{\rm hole}$ increase, because stripe fluctuations are reduced. However, the difference Δ decreases, because the hole's kinetic energy is enhanced by the additional tilt. Figure 6 shows Δ for finite system sizes, compared to respective ED results of ref. [2], and their extrapolation to $L_x \to \infty$. The variational energy is, of course, an upper bound to the true energy of the system. In the ED of ref. [2], $E_{\rm hole}$ was minimal for stripes with slightly tilted boundary conditions ($b = 2$ for even L_x, $b = 3$ for odd L_x). This suggested that the hole tends to bind to a kink in the stripe in order to increase its kinetic energy, at the expense of stripe fluctuations, forming a polaron. In our variational calculation, we observed the same effect for small system sizes (up to $L_x \approx 10$); however, for

TABLE I – *Variational and ED ground-state probabilities for* $(10, 0) \times (0, 7)$. *All other states, except those related by symmetry to the ones presented, have probability of less than* 1%.

Basis state	$\chi_{00}^{\downarrow\downarrow}$	$\chi_{01}^{\downarrow\uparrow}$	$\chi_{11}^{\downarrow\uparrow}$	$\chi_{11}^{\downarrow\downarrow}$	$\chi_{02}^{\downarrow\downarrow}$
Variational	23.4%	13.7%	4.3%	2.9%	1.4%
ED	19.2%	12.3%	4.7%	3.6%	1.8%

larger systems, the minimum energy is for $b = 0$ (1) for even (odd) L_x. This indicates that the preference for tilted boundary conditions, as observed in ED, may be only a finite-size effect. We also calculated the hole dispersion. On an untilted stripe, we find an effective mass $m_h^* = 6.43m^*$, where $m^* = 0.5$ is the mass of a non-interacting particle hopping on the lattice. This agrees remarkably well with ED, which gives $m_h^* \approx 6.7m^*$ [2]. If a hole would be forced to move only on the "main path", its effective mass would be $7.35m^*$. When the stripe has an overall tilt, the hole mass is reduced significantly, *e.g.* at $\mathrm{d}y/\mathrm{d}x = 0.5$, $m_h^* = 4.57m^*$.

A good measure of the coupling between the hole and the stripe is p_{main}, the ground-state probability of being in one of the "main path" basis states. In the variational ground state for an untilted stripe, we find $p_{\text{main}} = 0.91$, *i.e.* the hole tends to be decoupled from the stripe configuration. This probability is reduced as the stripe tilt increases and it is easier for the brackets to move from the hole (see fig. 5). This trend is supported by ED calculations, but the variational values for p_{main} are higher by up to 0.1. Comparison of the variational and ED ground states reveals that our calculation does a good job of qualitatively capturing the composition of the exact ground state from the basis set (*e.g.*, table I), but it overestimates the weight of states with low $l + r$.

In summary, we calculated the energy and the ground state for a single hole on a stripe, using a mapping to one dimension and a variational wave function constructed to decouple the hole and stripe degrees of freedom. We did not find evidence that the hole binds to a kink in the stripe, in the untilted case, for $L_x \gtrsim 10$.

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