Spontaneous currents in spinless fermion lattice models at the strong-coupling limit

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What kind of lattice Hamiltonian manifestly has an ordered state with spontaneous orbital currents? We consider interacting spinless fermions on an array of square plaquettes, connected by weak hopping; the array geometry may be a $2 \times 2L$ ladder, a $2 \times 2 \times 2L$ "tube," or a $2L \times 2L$ square grid. At half filling, we derive an effective Hamiltonian in terms of pseudospins, of which one component represents orbital currents, and find the conditions sufficient for orbital current long-range order. We consider spinfull variants of the aforesaid spinless models and make contact with other spinfull models in the literature purported to possess spontaneous currents.

DOI: 10.1103/PhysRevB.80.085116

PACS number(s): 71.10.Fd, 71.10.Hf, 71.10.Pm

I. INTRODUCTION

In condensed-matter physics, strongly correlated electrons underly a great variety of ordered states, both common and exotic (e.g., ferromagnets, superconductors). One of the lesser-studied orders is spontaneous currents (known sometimes as "orbital antiferromagnetism"). In this paper, we seek a *minimal* (spinless) toy model that manifestly exhibits such currents, precisely because any systematic study of fermion orderings with a quadratic order parameter reveals that the possible ordered states include not only the familiar cases of charge- or spin-density waves or superconductivity, but also spontaneous orbital currents.^{1–5} Yet such states have not been definitively observed in any material, nor numerically in the Hubbard model,⁶ and only very recently for any realistic microscopic Hamiltonian.^{7,8} Thus, we ask: which aspects of the interactions and/or degrees of freedom dispose a system generically toward ordered states with spontaneous currents ?

Such states were considered especially in the context of high- T_c cuprates. Early in their history, "flux phases" with current order were invented^{9–11} however the actual phase was expected to be disordered. More recently, two different kinds of spontaneous-current order were advanced to explain the mysterious pseudogap state of high- T_c cuprates.^{3,5} Reference 5 proposed the "*d*-density wave," which breaks translational symmetry (currents circulate in opposite senses around even and odd plaquettes); variants were considered more recently,¹² e.g., modulated versions.^{13,14}

In contrast, Varma's phases^{3,15} require the so-called "three-band" model in which oxygen orbitals of the CuO₂ layer are explicit independent degrees of freedom; the latter state breaks fourfold rotational and time-reversal symmetry but not translational symmetry. Experiments on photoemission¹⁶ (in BSCCO) and neutron diffraction¹⁷ (in YBCO) indicated time-reversal symmetry breaking, in the pattern of Ref. 15. Finally, Khomski and collaborators showed currents are implied by noncoplanar spin order in (spinfull) Mott insulators.¹⁸

These proposals motivate a basic question: under what circumstances, in principle, can a quantum state be realized with spontaneous currents? Where, in a model's parameter space, is such a state favored? Ever since the Hubbard model, toy lattice models, having a minimal parameter space and possibly amenable to solution, have been key tools to sort out basic questions such as these. For the more familiar orders, "strong-coupling" models are well known in which some "zero-order" state trivially has the order in question, and the order is stable against small perturbations. Thus, in the phase diagram, one is assured of a corner where the ordered phase occurs and extends an undetermined distance toward the regime where perturbations are large (which is usually the physical regime). But in the case of currents order, no general intuitive picture has emerged.

This paper addresses this question using a toy model built from square plaquettes; focusing mainly on the simplest case of *spinless* fermions, we explore the possibilities for realizing spontaneous currents. The main prior study of orbital currents in spinless models is Nersesyan's ladder model^{19,20} in which a map to spinfull chains was introduced that we adopt in Sec. IV B. Quite recently, spinless models were motivated by the possible realization in cold dilute atoms.²¹

The choice of square plaquettes is a choice motivated both by convenience of calculation and real-material geometries. As we will see, a square plaquette has spontaneous currents as one of its natural degrees of freedom which is what we desire to investigate: possibility of spontaneous currents in the zero-order ground state.

This paper is organized as follows: In Sec. II, we define our toy-model Hamiltonian and set up the various lattice geometries-tube, ladder, and square lattice-we shall deal with; we go on to describe the properties of one square plaquette as it forms the basic unit of all the lattice geometries considered, in particular, reducing its degrees of freedom to a pseudospin via the method of canonical transformations (which is briefly summarized in the Appendix, as it is the basis of all our subsequent calculations.) The core section is Sec. III, where we implement the pseudospin projection (illustrating it in detail for the case of a "tube" lattice) and obtaining a pseudospin effective Hamiltonian, showing its final form for the respective lattices; we also explore the relation between the fermion Hamiltonian and the pseudospin Hamiltonian, focusing on possibility of spontaneous currents in the ground state. In Sec. IV, we connect our work to spinfull models in two ways: simply incorporating spin (Sec. IV A) or mapping a pair of site indices to spin labels (Sec. IV B). At last in Sec. V we ask if we have learned how to construct a uniform lattice model with currents. We con-



FIG. 1. Geometry of a (a) tube, (b) ladder, and (c) square lattice. The fermions reside on the vertices of the lattices shown.

clude (Sec. VI) by discussing why it is hard to obtain spontaneous current order and what light this may shed on realistic motivated models of such order.

II. MICROSCOPIC MODEL AND PSEUDOSPIN MAPPING

Our basic model Hamiltonian is $\mathcal{H} = \mathcal{H}^{hop} + \mathcal{H}^{V} + \mathcal{H}^{V}$ with

$$\mathcal{H}^{\text{hop}} \equiv -t \sum_{\text{n.n.}\square} [c^{\dagger}(\mathbf{r})c(\mathbf{r}') + \text{H.c.}], \qquad (2.1a)$$

$$\mathcal{H}^{V} \equiv + V \sum_{\Box} \hat{n}(\mathbf{r}) n(\mathbf{r}'), \qquad (2.1b)$$

$$\mathcal{H}' \equiv -t' \sum_{\mathbf{n}.\mathbf{n}.\Box-\Box} \left[c^{\dagger}(\mathbf{r}) c(\mathbf{r}') + \text{H.c.} \right].$$
(2.1c)

Each site **r** has an orbital with room for one spinless fermion. A disjoint set of plaquettes ("strong plaquettes") are singled out. Within each strong plaquette (tagged by " \Box " in notations) there is a hopping -t on every bond; there is also a repulsion *V* between *any* two fermions (whether first or second neighbors in a spinless model, of course, there can be no onsite term).

Finally, every bond between bold plaquettes has a hopping -t', which is assumed to be a small perturbation. We will consider three kinds of lattice geometries, as shown in Fig. 1(a) a one-dimensional tube where the strong plaquettes are oriented transverse; (b) a ladder in which every other plaquette is strong, and (c) a square lattice in which one of four plaquettes is strong. The ladder is simplest but also has the least symmetry.

We were guided by three considerations while concocting the model of Eq. (2.1). First, we desired the spontaneous currents to be *explicitly* related to the degrees of freedom describing our (degenerate) ground state subspace. (See Sec. II B, below.) Second, the (zero-temperature) behavior should be obvious in a strong-coupling limit. A standard trick^{22,23} to achieve both ends is to artificially weaken some bonds thereby introducing a small parameter (t' in our case). In the t'=0 limit, the system decomposes into small disjoint clusters, each with a degenerate ground state whose operators are represented by pseudospins. As the small parameter is perturbatively turned on, it generates an effective Hamiltonian between the pseudospins; from the symmetry of the effective Hamiltonian, one can often read off the symmetry of its ground state.

TABLE I. States with n^{\Box} fermions on a plaquette.

n^{\Box}	Label	Occupation	Energy
0			0
1	$ 1\rangle$	$ \widetilde{0}\rangle$	-2t
2	$ 2+\rangle$	$ \widetilde{0},+\widetilde{1}\rangle$	-2t+V
	$ 2-\rangle$	$ \widetilde{0},-\widetilde{1} angle$	-2t+V
3	3>	$ \tilde{0},+\tilde{1},-\tilde{1}\rangle$	-2t+3V
4	$ 4\rangle$	$ \widetilde{0},+\widetilde{1},-\widetilde{1},\widetilde{2}\rangle$	6V

Finally, to make our model more physical, we limit the terms to fermion hoppings and interactions and no other four-fermion terms. Also, as we hope that our model(s) might later be adiabatically connected to a uniform one (see Sec. V), if a certain term is included (say) within strong plaquettes, we will be open to including an interplaquette term of the same form (with arbitrary coefficients). But we never assume any particular condition on the ratios between the intraplaquette and interplaquette terms, except that all of the latter are small for perturbation purposes.

A. Eigenstates of disconnected plaquettes

Let \mathcal{H}_0 include the \mathcal{H}^{hop} and \mathcal{H}^V terms, representing a set of disconnected squares. We will work at half filling, i.e., two fermions per square on average but our Hilbert space includes all ways of distributing these over the plaquettes.

Consider an isolated strong plaquette with sites x = 0, 1, 2, 3 forming a ring. Note \mathcal{H}_{\Box}^{V} is the same for all states accessible by hopping, so if there are n^{\Box} fermions on the plaquette, $\mathcal{H}_{\Box}^{V} = \frac{1}{2}n^{\Box}(n^{\Box} - 1)V$ drops out like a *c* number: as in a noninteracting model,²⁴ multifermion states are built from the one-particle eigenstates on the ring, defined by creation operators

$$\tilde{c}_m^{\dagger} \equiv \frac{1}{2} \sum_{x} e^{1/2i\pi mx} c^{\dagger}(x), \qquad (2.2)$$

where $m=0, \pm 1, 2$ is the angular momentum around the ring. The single-fermion eigenenergies are

$$E_m = -2t\cos\left(\frac{1}{2}\pi m\right),\tag{2.3}$$

i.e., $E_0 = -2t$, $E_{\pm 1} = 0$, $E_2 = +2t$. Table I lists the multifermion ground states for each occupation sector of a single plaquette. Our interest will be the two-fermion sector since it has degenerate ground states $|2+\rangle$ and $|2-\rangle$ with spontaneous current in the + and – senses, respectively.

To have any possibility of a symmetry-broken state, (at least some of) the plaquettes must be in the degenerate half-filled ground states. What is the ground state of an extended system of *N* sites forming *N*/4 disconnected plaquettes with *N*/2 fermions (i.e., half filling)? The case *V*=0 is more degenerate than we wished since any combination of states with $n^{\Box}=1,2,3$ has total energy -2t(N/4). However, taking *V*>0 favors the subspace in which $n^{\Box}=2$ on every plaquette.

In that case, the only freedom is the senses of the currents in each of the N/4 plaquettes, giving a degeneracy $2^{N/4}$.

B. Pseudospin mapping

These states can be labeled as an array of spin- $\frac{1}{2}$ pseudospins \vec{P}_{α} with $P_{\alpha}^{z} = \pm 1/2$ when plaquette α is in state $|2\pm\rangle$. We aim, via second-order perturbation in t', to compute the effective Hamiltonian \mathcal{H}_{σ} defined within the ground-state manifold (and thus taking the form of a spin Hamiltonian in $\{\vec{P}_{\alpha}\}$.)

The spin- $\frac{1}{2}$ pseudospin Hilbert space can be defined as follows:

$$|\pm\rangle_{z} \equiv |\pm\rangle \equiv |2\pm\rangle,$$

$$|\pm\rangle_{x} \equiv \frac{1}{\sqrt{2}}(|2\pm\rangle\pm|2\pm\rangle),$$

$$|\pm\rangle_{y} \equiv \frac{1}{\sqrt{2}}(|2\pm\rangle\pm i|2\pm\rangle).$$
(2.4)

Different orders of the fermions—spontaneous currents and (site- or bond-centered) charge-density waves correspond to expectations of three characteristic operators; when projected to the pseudospin subspace, Eq. (2.4), these reduce to the three pseudospin operators (here i, j=0, ..., 3label sites counterclockwise around a plaquette, as in Figs. 3 and 4)

Pseudocurrent operator

$$\hat{I}_{ij} = -\hat{I}_{ji} \equiv i(c_i^{\dagger}c_j - c_j^{\dagger}c_i) \to \frac{\hat{P}^z}{2}.$$
 (2.5a)

Charge-density operator

$$\hat{n}_i \equiv c_i^{\dagger} c_i \to (-1)^i \frac{\dot{P}^x}{2} + \frac{1}{2}.$$
 (2.5b)

Bond-density operator

$$\hat{B}_{ij} \equiv (c_i^{\dagger}c_j + c_j^{\dagger}c_i) \to -(-1)^{(i+j)}\frac{\hat{P}^y}{2} + \frac{1}{2}.$$
 (2.5c)

Here " \rightarrow " means the operators have the same matrix elements when acting in the pseudospin Hilbert space. Any operators in the pseudospin subspace of a plaquette can be expressed in terms of $\vec{P} \equiv (\hat{P}^x, \hat{P}^y, \hat{P}^z)$. Figure 2 depicts states in which the respective operators have expectations.

So, for purposes of nomenclature, we call the pseudospin states in the z direction as current carrying states (which is expected since +1 and -1 carry momentum) or CCS, the pseudospin states in the x direction as charge-density waves or CDW, and the pseudospin states in the y direction as bond-density waves or BDW. Spontaneous currents, orbital currents, or just currents will be used interchangeably to refer to CCS as they have been used in the literature before. (The "bond order," making different directions inequivalent without a translational modulation of the charge density, would



FIG. 2. Properties of single plaquette eigenstates. Arrows represent orbital currents. Lines represent the bond density; nondashed line represents unit bond density, dashed line represents half, and absence of line represents zero bond density. The numbers at the corners of the plaquette represent the charge density at the respective sites. Note that they add up to two corresponding to half filling.

be an example of "electron nematic"^{25,26} if all similarly oriented bonds had the same order parameter.)

Incidentally, we use the term *pseudo*current operator because this is not the true current operator. The latter would be the time derivative of the charge-density operator and is evaluated as a commutator of the charge-density operator with the full Hamiltonian. Most often, the true current is proportional to (or at least has overlap with) the pseudocurrent operator; then, any state with pseudocurrent order will also have true current order. (The pseudocurrent would be the real current if the Hamiltonian contained only nearestneighbor hopping.)

III. EFFECTIVE PSEUDOSPIN HAMILTONIAN

In this section, we go on to calculate an effective Hamiltonian by second-order perturbation theory formulated via canonical transformations (reviewed briefly in Appendix.). We shall consider several variations on the model Hamiltonian (2.1); the result is always a special case of the general form

$$H_{\sigma} = \sum_{\langle \alpha\beta\rangle} \left[J_x P^x_{\alpha} P^y_{\beta} + J_y P^y_{\alpha} P^y_{\beta} + J_z P^z_{\alpha} P^z_{\beta} \right] - \sum_{\alpha} \left[h_x P^x_{\alpha} + h_y P^y_{\alpha} + h_z P^z_{\alpha} \right].$$
(3.1)

Here P_{α} is the pseudospin; (α runs over all strong plaquettes and $\langle \alpha \beta \rangle$ are nearest neighbors (in the ladder, tube, or square-lattice arrangements). In view of the mapping of operators, Eq. (2.5), the original system has spontaneouscurrent order if and only if Eq. (3.1) has pseudospin order in the *z* direction. Consequently, our central concern is whether and how the terms in Eq. (3.1) break pseudospin rotation symmetry.

The above form of the effective Hamiltonian is governed by the two different kinds of interplaquette hopping processes that can occur at second-order perturbation theory. As



FIG. 3. The two-plaquette unit involved in a second-order hopping process. Site labels show our convention for the tube.

we will see in the next subsection, at second order, only two adjoining plaquettes can take part in the hopping processes. On the one hand, a "degenerate" hop takes a fermion from a plaquette to a single-fermion orbital on the adjoining plaquette, degenerate with the orbital it hopped out of; such hops are responsible for all the pseudospin exchange interactions.

On the other hand, an "excited" hop takes a fermion from a plaquette to a single-fermion orbital on the adjoining plaquette, that is, not degenerate with the orbital it hopped out of. The only way to return to the degenerate pseudospin manifold is to undo the same hop thus making exchange of pseudospins impossible. Consequently, excited-state hops can (at most) generate only single-pseudospin terms in the effective Hamiltonian.

We shall first consider the tube model case (Sec. III A) since it has the greatest symmetry (the combination of two adjoining plaquettes has a fourfold rotation). The other two cases (Sec. III B) are variations on the tube case, in that either additional terms appear (due to reduced symmetry) or are accidentally canceled.

A. Effective Hamiltonian for the tube

The perturbation (t' hopping) changes the filling on two plaquettes, hence no first-order process stays in the reduced Hilbert space (of $n_{\alpha}^{\Box}=2$ on all plaquettes). To do that in a second-order process, a fermion hops from one plaquette (A) to a neighboring one (B) and then a fermion hops back from the second to the first plaquette.

For a pair of plaquettes on a tube (Fig. 3), the perturbation takes the form

$$\mathcal{H}' = -t' \left(\sum_{i} c^{\dagger}_{A,i} c_{B,i} + \text{H.c.} \right) = -t' \left(\sum_{m} \widetilde{c}^{\dagger}_{A,m} \widetilde{c}_{B,m} + \text{H.c.} \right).$$
(3.2)

Notice that the hopping conserves the angular momentum around the plaquette. For this reason, the only excited states that can participate in the second-order hopping processes are $|1;3\rangle \equiv |\tilde{0};\tilde{0},+\tilde{1},-\tilde{1}\rangle$ and $|3;1\rangle \equiv |\tilde{0},+\tilde{1},-\tilde{1};\tilde{0}\rangle$ and the corresponding nonzero matrix elements are

$$\langle 1; 3 | \mathcal{H}' | 2 + ; 2 - \rangle = t'$$

$$\langle 3; 1 | \mathcal{H}' | 2 + ; 2 - \rangle = t'$$

$$\langle 1; 3 | \mathcal{H}' | 2 - ; 2 + \rangle = -t'$$

$$\langle 3; 1 | \mathcal{H}' | 2 - ; 2 + \rangle = -t'.$$

The rest of the matrix elements are zero. Thus, using Eq. (A1), we get the following second-order effective two-plaquette Hamiltonian

$$H_{tube} = -\frac{2t'^2}{V}(|2+;2-\rangle\langle 2+;2-|+|2-;2+\rangle\langle 2-;2+|) + \frac{2t'^2}{V}(|2+;2-\rangle\langle 2-;2+|+|2-;2+\rangle\langle 2+;2-|).$$
(3.3)

Conversion to spin Hamiltonian: In accord with our pseudospin mapping, we abbreviate $|2\pm\rangle$ by $|\pm\rangle$ to label the pseudospin states. Now, the transcription to spin notation [for pseudospin (*P*)] is

$$|2+\rangle\langle 2+| \rightarrow \left(\frac{1}{2} + P^{z}\right);$$

$$|2-\rangle\langle 2-| \rightarrow \left(\frac{1}{2} - P^{z}\right);$$

$$|2+\rangle\langle 2-| \rightarrow P^{+};$$

$$|2-\rangle\langle 2+| \rightarrow P^{-}.$$
(3.4)

Inserting Eq. (3.4) into Eq. (3.3), we get for the infinite tube

$$H_{tube} = \sum_{\alpha} \frac{4t'^2}{V} \left[\frac{1}{4} + \vec{P}_{\alpha} \cdot \vec{P}_{\alpha+1} \right].$$
(3.5)

Thus, the effective pseudospin Hamiltonian for the tube is a one-dimensional spin-1/2 Heisenberg antiferromagnet which, as is well known, does not exhibit long-range order but only power-law correlations.

This calculation is not only reminiscent of, but completely analogous to, the derivation of the effective Heisenberg antiferromagnetic exchange interaction in a half-filled Hubbard model; the role of spin is taken by our angular momentum, since it is conserved by the hopping along the tube. Hence only our $|\pm \tilde{1}\rangle$ single-particle states (analogous to spin-up and spin-down electrons) take part in the second-order process, thus giving rise to effective pseudospin exchange of exactly the same (rotationally symmetric) form as spin exchange in the Hubbard model. This is exactly the content of the discussion on degenerate hops in Sec. III.

In other cases of our model (ladder or square lattice), the perturbation need not conserve angular momentum, so excited states such as $|\tilde{0}; \tilde{0}, +\tilde{1}, \tilde{2}\rangle$ or $|\pm \tilde{1}; \tilde{0}, +\tilde{1}, -\tilde{1}\rangle$ may then mediate second-order processes via the "excited-state" hops defined at the beginning of this section Thus, they will give rise to single-site pseudospin terms only.

B. Ladder and square lattice

In this subsection, we list down the results of similar calculations for ladder and square lattice cases. For the ladder, the effective pseudospin Hamiltonian is

$$H_{ladder} = \sum_{\alpha} -\frac{t'^2}{V} \left[P_{\alpha}^z P_{\alpha+1}^z - \frac{1}{2} (P_{\alpha}^+ P_{\alpha+1}^+ + P_{\alpha}^- P_{\alpha+1}^-) \right] + \frac{t'^2}{2V} \left(\frac{1}{1+x} \right) (P_{\alpha}^y) + \text{const}, \qquad (3.6)$$

where $x \equiv 2t/V$. To make the symmetry of the above expression clear, we make a simple transformation as follows.

Staggered pseudospins: Let us define a new set of staggered spin operators \vec{T}_{α} , by switching the definitions of "up" and "down" pseudospin on every other site *B* by a 180° rotation around *y* axis. Then,

$$P_B^z \to -T_B^z;$$

$$P_B^x \to -T_B^x;$$

$$P_B^y \to T_B^y;$$

$$P_A^\pm \to T_B^{\mp}$$
(3.7)

while pseudospin operators on sites A stay unchanged. This transformation converts Eq. (3.6) to

$$H_{\sigma} = \sum_{\alpha} \left\{ \frac{t'^{2}}{V} [\text{const}(x) + \vec{T}_{\alpha} \cdot \vec{T}_{\alpha+1}] + \frac{t'^{2}}{2V(1+x)} T_{\alpha}^{y} \right\}.$$
(3.8)

In Eq. (3.8), there is a uniform magnetic field in the pseudospin y direction. We get the single-site terms from the excited hops (defined at the start of this section) which are not disallowed for the ladder. This competes with the anti-ferromagnetic exchange term, having the effect (as usual in antiferromagnets) of a uniaxial anisotropy favoring the *xz* plane. Hence, the system has the symmetry of an XY model ordering in that plane, which corresponds [by Eq. (2.5)] to CDW and spontaneous currents. Since this model is in one spatial dimension and has a continuous spin symmetry, it would only have power-law correlations (as we noted above for the tube case).

Doing the same for the square lattice amounts to extending the result of the ladder calculation to a square lattice. Recalling for the ladder [Eq. (3.8)], the pseudospin Hamiltonian for the two-plaquette unit was

$$H_{\sigma} = \frac{t'^{2}}{V} [\text{const}(x) + \vec{T}_{A} \cdot \vec{T}_{B}] + \frac{t'^{2}}{2V} \left(\frac{1}{1+x}\right) (T_{A}^{y} + T_{B}^{y}).$$
(3.9)

The similar result for the perpendicular direction in the plane would be

$$H_{\sigma} = \frac{t'^2}{V} [\text{const}(x) + \vec{T}_A \cdot \vec{T}_B] - \frac{t'^2}{2V} \left(\frac{1}{1+x}\right) (T_A^{y} + T_B^{y}).$$
(3.10)

The minus sign for the single-plaquette terms in the second case is because the bond ordering in the two perpendicular directions are the pseudospin in +y and -y directions, respec-

tively (see Fig. 2). Hence for the infinite square lattice, we get

$$H_{square} = \frac{t'^2}{V} \sum_{\langle \alpha, \beta \rangle} \left[\text{const}(x) + \vec{T}_{\alpha} \cdot \vec{T}_{\beta} \right]$$
(3.11)

which is the antiferromagnetic Heisenberg Hamiltonian. Since, the square lattice is two dimensional, its ground state will possess long-range order. Notice that antiferromagnetic tendency of staggered pseudospin implies a ferromagnetic tendency for spontaneous currents in both ladder and the square lattice.

C. Role of symmetries

Exploring symmetries can lead to a better understanding of the relation between the form of microscopic model and that of the effective Hamiltonian. Our starting fermion Hamiltonian (acting on a two-plaquette unit) had the following symmetries: (a) time reversal and (b) reflection symmetry (flipping the two plaquette upside down). We have only considered models that maintain these symmetries.

1. Consequences of generic symmetries

These symmetries imply specific symmetries in the pseudospin effective Hamiltonian (3.1). (a) The absence of a single-site term \hat{P}^z follows from the microscopic time-reversal symmetry under which the *pseudocurrent* operator flips sign. (b). The absence of a single-site term \hat{P}^x is due to the transverse reflection symmetry of the two-plaquette unit under which the *charge-density* operator flips sign.²⁷

The tube and square lattices both have a fourfold rotation symmetry, too, under which the two bond-order states (pseudospin +y and -y) are equivalent, ergo the \hat{P}^y terms are absent. Moreover, for the most general one-particle spectrum that a single plaquette could have (keeping intact the degeneracy of momentum carrying states, i.e., +1 and -1, but lacking particle-hole symmetry), the effective Hamiltonian would still be of form Eq. (3.8), though with different numerical coefficients. On the other hand, the effective Hamiltonian for the ladder generically includes single-site \hat{P}^y terms since they are not ruled out by any symmetry.

2. Role of lattice symmetry in ladder model

In our basic ladder Hamiltonian (2.1), the single-plaquette terms had an "accidental" (nongeneric) fourfold rotational symmetry not guaranteed by the ladder's symmetries. If we generalize the ladder model so as to break the fourfold symmetry, what kinds of pseudospin asymmetries are generated?

If we make the transverse hopping t_{\perp} within a strong plaquette different from the longitudinal *t*, then the effective Hamiltonian turns out to be

$$H_{ladder} = \text{const} + \sum_{\alpha} \left(\frac{t'^2}{2V} \right) \vec{T}_{\alpha} \cdot \vec{T}_{\alpha+1} + \left(\frac{t'^2}{2V} \right) \\ \times \left[\frac{2\Delta t}{(V - 2\bar{t} + \Delta t)(V - 2\bar{t} + 3\Delta t)} \right] T^y_{\alpha} T^y_{\alpha+1} \\ + \left[\frac{t'^2}{2(V - 2\bar{t} + 3\Delta t)} + 2\Delta t \right] T^y_{\alpha}, \quad (3.12)$$

where $\overline{t} \equiv (t+t_{\perp})/2$ and $\Delta t \equiv t_{\perp} - t$. The absence of fourfold symmetry of the hopping around the plaquette leads to a first-order field term $+2\Delta t T^y$ and a second-order anisotropic exchange along the T_y (BDW) pseudospin direction for the ladder. This is because angular momentum is not a good quantum number anymore, rather bond order is the good quantum number.

Alternatively, we could spoil the fourfold symmetry of *intra*plaquette interactions which produce single-pseudospin terms. Making transverse and longitudinal interaction different gives a linear coupling at first-order in perturbation theory to the bond-charge operator $\propto (V_{\parallel} - V_{\perp})T_y$; as before, the time reversal and reflection symmetries forbid linear T_x or T_z terms.²⁸

D. Engineering spontaneous currents by fermion interactions (ladder)

Our study was motivated by the question: can the microscopic models considered so far exhibit current-carrying states spontaneously in their ground state with genuine order in an Ising sense. To stabilize any particular kind of order more than the others, we must spoil the symmetries by anisotropic pseudospin terms having the effect of an Ising-type anisotropy in the desired direction.

In this section, we see if interplaquette interaction can achieve this. The simplest such perturbation we can add to Eq. (3.8) is the nearest-neighbor term

$$H' = V'[n_A(1)n_B(0) + n_A(0)n_B(1)].$$
(3.13)

We have used the ladder numbering scheme in writing the above expression. Looking at Fig. 2, we see how the term, Eq. (3.13), distinguishes the CDW sector from others, since the operators such as $n_A(1)$ depend on the CDW order; on the other hand, it cannot distinguish different CCS or BDW states, since they have equal fermion densities on all sites. Using Eq. (2.5), we can easily convert the interaction term to pseudospin language and indeed

$$H'_{\sigma} = V'\left(\frac{1}{2} - \frac{P_A^x P_B^x}{2}\right) = V'\left(\frac{1}{2} + \frac{T_A^x T_B^x}{2}\right).$$
 (3.14)

We emphasize the above effective interaction, Eq. (3.14), is *first* order in perturbation theory and not second order as for the hopping processes earlier in Sec. III. Equation (3.14) is an adjustment of the J_x pseudospin coupling in Eq. (3.1) and thus favors CDW order, either a uniform pattern on each plaquette or an alternating one, depending on the sign and magnitude of V'. An interplaquette second-nearest-neighbor interaction, i.e., $V''[n_A(0)n_B(0)+n_A(1)n_B(1)]$, gives the same



FIG. 4. The two-plaquette unit involved in a second-order hopping process for the ladder. Site labels show our convention for the ladder.

result as Eq. (3.14) but with a flipped sign for the exchange term.

Thus, we see a route to favoring spontaneous currents for the ladder. An infinitesimal attractive interplaquete secondnearest-neighbor interaction (V' < 0) or repulsive interplaquette second-nearest-neighbor interaction (V'' > 0) will make $J_z > J_x$ and the ground state will have currents spontaneously. For a comparison, we note that in generalized Hubbard models, attractive nearest-neighbor interaction was argued to stabilize currents.²⁹

For the tube and square lattice, interplaquette interactions can only reduce the antiferromagnetic Heisenberg symmetry to a continuous XY symmetry in currents/BDW plane and do not favor currents exclusively. To do that, we must look to interplaquette hoppings instead.

E. Engineering spontaneous currents by fermion hops (square lattice)

An alternative extension of our model is to add additional interplaquette hoppings. As we will see, for the ladder and square lattice, this favors bond (BDW) order by increasing the J_y pseudospin exchange while decreasing J_x and J_z couplings in Eq. (3.1). For the tube, interplaquette hopping to any distance can never reduce the continuous Heisenberg symmetry due to fourfold symmetry.

1. Guessing the fermion term?

A shortcut may allow us to quickly find fermion terms yielding a desired interplaquette pseudospin Hamiltonian form. Let's extend the notion of "pseudospin" backward to impute pseudospin to the single-fermion states $|\pm 1\rangle$. Indeed, we can just ignore the other orbitals since only the degenerate hoppings (explained at start of Sec. III) could give us a pseudospin interaction from second-order perturbation theory. Then, we just substitute $\vec{T}_A \rightarrow \sum_{\sigma'\sigma} c_{\sigma'}^{\dagger}(A) \vec{\tau}_{\sigma'\sigma} c_{\sigma}(A)$, where $\vec{\tau}_A$ means the usual Pauli matrices. Thus, any coupling $\mathcal{H}_{\text{eff}}^T$ between (components of) pseudospins \vec{T}_A and \vec{T}_B gets transcribed to a four-fermion term $\mathcal{H}_{\text{eff}}^c \simeq -\hat{\mathcal{H}}'^{\dagger}\hat{\mathcal{H}}'$ where the operator $\hat{\mathcal{H}}'$ hops a fermion from plaquette *B* to *A*, then we could take $\hat{\mathcal{H}}'$ to be the interplaquette term reducing to $\mathcal{H}_{\text{eff}}^c$ via second-order perturbation theory.

When applied to two plaquettes in a ladder or square lattice (using the site labels of Fig. 4), we get SPONTANEOUS CURRENTS IN SPINLESS FERMION ...

$$T_A^{\mathfrak{c}}T_B^{\mathfrak{c}} + T_A^{\mathfrak{y}}T_B^{\mathfrak{y}} \longrightarrow (c_{A,1}^{\dagger}c_{B,0})(c_{A,0}c_{B,1}^{\dagger}) + (A \leftrightarrow B), \quad (3.15)$$

where there was only one grouping such that the interplaquette hops connected nearest neighbors; this is precisely the nearest-neighbor weak hopping, Eq. (2.1c). What about the term which would break the degeneracy between bond order and pseudocurrents

$$-T_A^{\varepsilon}T_B^{\varepsilon} + T_A^{\gamma}T_B^{\gamma} \to (c_{A,0}^{\dagger}c_{B,0})(c_{A,1}c_{B,1}^{\dagger}) + (A \leftrightarrow B).$$
(3.16)

The grouped factors in Eq. (3.16) are diagonal $(t'_{\sqrt{2}})$ fermion hops. Unfortunately, the sign of this term is necessarily positive, so it always favors the T_y (bond-order) direction in pseudospin space.

2. Fermion hops in general

A more comprehensive study of hops will be profitable for the following reasons: (i) as we are about to show, it reveals that the findings in Eqs. (3.15) and (3.16) are general for any nearest-neighbor hopping, so that is not a route to the desired order. (ii) Consequently, further-neighbor pseudospin interactions coming from long-distance fermion hops are our last hope to disfavor bond order in the square lattice and the general formula guides us to the correct interactions for this purpose. (iii) It is the root reason that the ladder and squarelattices' pseudospins needed to be staggered but not the tube lattice's.

Imagine a perturbation Hamiltonian containing hops from *any* vertex of one strong plaquette to any vertex of another. Let t'_1 , $t'_{\sqrt{2}}$, t'_2 , etc. be weak hoppings to sites at distances 1, $\sqrt{2}$, 2, and so on, respectively. Then the exchange part of the two-plaquette effective pseudospin Hamiltonian is

$$H_{\sigma} = J_{T}\vec{T}_{A} \cdot \vec{T}_{B} + J_{P}\vec{P}_{A} \cdot \vec{P}_{B}$$

= $(J_{T} + J_{P})P_{A}^{y}P_{B}^{y} - (J_{T} - J_{P})(P_{A}^{z}P_{B}^{z} + P_{A}^{x}P_{B}^{x}),$
(3.17)

where

$$J_T = (t_1' - 2t_{\sqrt{5}}' + t_3')^2 / V > 0, \qquad (3.18a)$$

$$J_P = (t'_{\sqrt{2}} - 2t'_2 + t'_{\sqrt{10}})^2 / V > 0.$$
 (3.18b)

Which kind of exchange does a given hopping give rise to? If we orient the two plaquettes such that the two hoppings do not cross, the exchange coupling relates staggered pseudospins or plain pseudospins depending on whether clock sense of the numbering scheme on the two plaquettes are same or alternating respectively (e.g., in Fig. 4, the noncrossed hoppings are connecting plaquettes with same clock sense, thus giving rise to staggered pseudospin exchange coupling, i.e., $\vec{T}_A \cdot \vec{T}_B$).

A related observation is that, in the ladder, there is a symmetry under mirror flipping every second plaquette around the long axis of the ladder, while switching $t'_1 \leftrightarrow t'_{\sqrt{2}}$ and $t'_2 \leftrightarrow t'_{\sqrt{3}}$; Eq. (3.18) shows this switches the \vec{T} and \vec{P} terms.

Inspecting Eq. (3.17), we see that so long as we have only crossed or only uncrossed fermion hoppings, the result is

isotropic in the (yz) pseudospin plane, so that bond order and currents are degenerate. However, if we start from a mixture of crossed and uncrossed hoppings, the bond-order (y) exchange is always stronger than the currents (z) exchange—and is always antiferromagnetic.

3. Spontaneous currents via anisotropic frustration

Given this last fact, is it possible at all to obtain a pseudospin anisotropy favoring T_z and hence current order over the whole lattice, by coupling more distant units? This is possible, in principle, through *anisotropic frustration*. (It is assumed interactions have somehow already disfavored charge ordering, as discussed in Sec. III D.)

Assume the dominant nearest-neighbor hopping is purely t'_1 , as in our original and simplest model. The pseudospin exchange has a continuous symmetry in the yz spin plane leading to antiferromagnetic order degenerately in any mixture of those components. Now imagine (say) a second-neighbor pseudospin exchange due to mixed kinds of hoppings; by the above arguments, J_{2y} is necessarily antiferromagnetic, and $J_{2y} > |J_{2z}|$. But unlike the nearest-neighbor exchange, the enhanced second-neighbor J_{2y} term *disfavors* bond-order state (being of the wrong sign).

A second-neighbor exchange is allowed on the ladder, using (say) the hops t''_3 and $t''_{\sqrt{10}}$ connecting two plaquettes related by a [4,0] vector. On the square lattice, the second nearest neighbor has a displacement [2,2] and this exchange turns out to be symmetry forbidden. But the square lattice can have the same [4,0] interplaquette hops as on the ladder and these finally give our goal: we can favor spontaneous order in the square lattice, albeit with a rather baroque Hamiltonian.

IV. GENERALIZATION TO SPINFULL MODELS

It is natural to ask if we can extend our results to models with spin. There are two quite different ways to imagine this. First, as worked out in Sec. IV A, we can simply include an additional spin degree of freedom in the Hamiltonians considered above. Alternately, as worked out in Sec. IV B we can exactly map a site degree of freedom in one of our spinless models to the spin degree of freedom in a model with half as many of lattice sites (thus keeping constant the total degrees of freedom.)

A. Adding spin degree of freedom

For this extension of our model, we simply add spin indices in all the terms of Eq. (2.1) while conserving the spin and rerun the calculations of Secs. II and III. To make the spinfull calculation analogous to what we did, the filling should now be 3/8. Of the three fermions per plaquette, the first two fill angular momentum zero $(|\tilde{0}\uparrow\rangle$ and $|\tilde{0}\downarrow\rangle$). The third fermion goes in the degenerate current-carrying state, $|\pm \tilde{1}\sigma\rangle$. The extended pseudospin representing each plaquette is now the direct product of the same pseudospin degree of freedom and a real spin \vec{S}_{α} .³⁰ Also, the interaction term in Eq. (2.1b) has to be augmented to include an onsite interaction term (U) equal in strength to the offsite interaction terms (V) so that the multifermion eigenstates still remain direct products of single-fermion orbitals.

Here are the results for each case: Spinfull tube

$$\begin{split} H_{\rm eff} &= \left(\frac{2t'^2}{V}\right) \sum_{\alpha} \left[(\vec{P}_{\alpha} \cdot \vec{P}_{\alpha+1}) + (\vec{S}_{\alpha} \cdot \vec{S}_{\alpha+1}) \right. \\ &+ 4(\vec{P}_{\alpha} \cdot \vec{P}_{\alpha+1}) (\vec{S}_{\alpha} \cdot \vec{S}_{\alpha+1}) \right]. \end{split} \tag{4.1}$$

Spinfull ladder

$$H_{\rm eff} = \left(\frac{t'^2}{2V}\right) \sum_{\alpha} \left[\left(\frac{1}{2}\right) \vec{T}_{\alpha} \cdot \vec{T}_{\alpha+1} + (\vec{T}_{\alpha} \cdot \vec{T}_{\alpha+1}) (\vec{S}_{\alpha} \cdot \vec{S}_{\alpha+1}) - \left(\frac{1}{1+x}\right) T_{\alpha}^{y} \right].$$

$$(4.2)$$

Spinfull square lattice

$$H_{\rm eff} = \left(\frac{t^{\prime 2}}{2V}\right) \sum_{\langle \alpha, \beta \rangle} \left[\left(\frac{1}{2}\right) \vec{T}_{\alpha} \cdot \vec{T}_{\beta} + (\vec{T}_{\alpha} \cdot \vec{T}_{\beta}) (\vec{S}_{\alpha} \cdot \vec{S}_{\beta}) \right].$$

$$(4.3)$$

Thus the effective Hamiltonians have a form such as the Kugel-Khomskii³¹ Hamiltonian for cubic titanates describing spin and orbital superexchange interactions between d^1 ions having threefold degenerate t_{2g} orbitals.

The result, Eq. (4.1), for the tube case is proportional (modulo a constant) to $(\frac{1}{2}+2\vec{P}_{\alpha}\cdot\vec{P}_{\alpha+1})$ $(\frac{1}{2}+2\vec{S}_{\alpha}\cdot\vec{S}_{\alpha+1})$ which is the SU(4) symmetric Kugel-Khomskii model.³² For the tube, the interaction terms are just degenerate hops of Sec. III; they conserve spin as well as pseudospin. Actually, they conserve a combined flavor which includes both the spin and the pseudospin. Hence, the effective Hamiltonian possesses an SU(4) symmetry in which there is no distinction between the four combined flavors the hopping fermion might carry. The interesting behavior of such SU(4) chains is discussed in Ref. 32; in terms of the original fermions, it obviously corresponds to a high degeneracy between many kinds of order.

For the ladder and square lattice cases, the degenerate hops do not conserve the combined flavor thereby reducing the SU(4) symmetry to only SU(2) × SU(2) for the exchange terms. What kind of order do these lattices have? Notice that the spin-pseudospin cross terms tend to favor ferromagnetic order in one kind and antiferromagnetic order in the other. Since we also have a pseudospin antiferromagnetic exchange but no real spin exchange, the expected order is always *ferromagnetic* for the real spins.³³ Then the pseudospin order is the same as in a spinless model; in effect, the system spontaneously becomes spinless by polarizing in one spin flavor.

We compare our results to that of Ref. 35, in which a Hubbard model with a similar pattern of strong and weak plaquettes (t and t') with just an onsite interaction term was studied on a square lattice. Yao *et al.* found a host of different phases for different values of the onsite interaction including a Fermi liquid, a *d*-BEC (Bose Einstein condensate), a *d*-CDW, a *d*-BCS, a spin-1/2 antiferromagnet, a spin-3/2 antiferromagnet, and an "orbital nematic" phase at 3/8 fill-

ing, which is equivalent to one doped hole with respect to half filling, on each plaquette (" $Q_h=1$ " or "x=1/4" in their notation). In their model, it is only the parameter regime $U_c \approx 4.6t < U < U_t \approx 18.6t$ which admits the possibility for currents.³⁴ Then, the single-plaquette states are characterized by spin-1/2 as well as a pseudospin-1/2 (called chirality τ_z by Ref. 35, and having " $p_x \pm ip_y$ " symmetry, i.e., our angular momentum $|\pm \tilde{1}\rangle$.)

The possibilities of orbital currents are not explicitly discussed in the above mentioned regime but implicit in the results are the anisotropies in the pseudospin exchange terms which is interesting [see Eqs. (4) and (6) of Ref. 35]. In the regime $U_c < U < U_n \approx 7.3$, the system becomes a spin-1/2 antiferromagnet with electron nematic order (same as our BDW), while in $U_n < U < U_t$, there is no nematic ordering. Perhaps, there are spontaneous currents in this regime. However, they do not discuss the origin of the pseudospin anisotropies. It is all the more perplexing to us, given our experience that one set of degenerate hops taking part in the second-order perturbation theory can only give rise to isotropic exchange.

B. Nersesyan map

As first proposed by Nersesyan,¹⁹ a spinfull model on any lattice can be mapped to a spinless model on a doubled version of that lattice (its direct product by $\{1,2\}$.) Each pair of sites in the spinless model represents, respectively, the spin-up and spin-down occupation. Thus, a spinless ladder maps to a spinfull chain (or vice versa), such that the leg index maps to the spin index. (We shall call this a "rung spin" to distinguish it from the real spin of Sec. IV A and the pseudospin of all the earlier sections.) Hamiltonian terms acting on a single rung of the ladder will be mapped to single-site terms on the chain while terms along the ladder's leg map to terms along the chain's leg. We exhibit examples of the map in both directions.

In fact, since our plaquette is built from two rungs, each plaquette pseudospin operator \vec{P}_i corresponds to two neighboring rung spin operators as shown below. Consider the fermion basis states on each rung *j* that have nonzero pseudocurrents, namely,

$$|\phi_{j+}\rangle \equiv (|j,1\rangle + i|j,2\rangle)/\sqrt{2}, \qquad (4.4a)$$

$$|\phi_{j-}\rangle \equiv (|j,1\rangle - i|j,2\rangle)/\sqrt{2}.$$
 (4.4b)

The \pm label in Eq. (4.4) is a rung pseudospin index defining the z axis for rung pseudospin \vec{S}'_j aligned with that of the plaquette pseudospin such that

$$\vec{S}'_{2j} = (P^x_j, P^y_j, P^z_j),$$
 (4.5a)

$$\vec{S}_{2i+1}' = (-P_i^x, P^y j, -P_j^z).$$
(4.5b)

On the other hand, Nersesyan's rung spins (we call \vec{S} keeping in mind the difference from the previous section) are related to our rung spins \vec{S}' via [see Eqs. (3)–(5) of Ref. 19]

$$S_i^x = (-1)^j S_i^{\prime y}, \tag{4.6a}$$

$$S_j^{y} = (-1)^j S_j^{\prime z},$$
 (4.6b)

$$S_i^z = (-1)^j S_i'^x. \tag{4.6c}$$

Notice that the definition of Nersesyan's rung spins is staggered compared to ours. Nersesyan used a "canted" rung spin basis to make manifest the staggered nature of charge/spin densities in CDWs and spin-density waves (SDW) for a spin-1/2 Hubbard chain. We will write rung spins using the Nersesyan basis from now on. Using Eq. (4.6), we can reuse the results of Sec. III to figure out what a given fermion perturbation projects to in terms of Nersesyan pseudospins.

As an illustration, our basic Hamiltonian for the spinless ladder [see Eq. (2.1)] gets mapped to a chain of alternating strong and weak bonds ("sf" here distinguishes the spinfull model parameters)

$$\mathcal{H} \equiv -\sum_{i,\sigma} t_{i,i+1}^{\text{sf}} [c_{i\sigma}^{\dagger} c_{i+1,\sigma} + \text{H.c.}] + U^{\text{sf}} \sum_{i} \hat{n}_{i\uparrow} n_{i\downarrow} - h_x^{\text{sf}} \sum_{i} S_i^{\lambda} + \sum_{i} V_{i,i+1}^{\text{sf}} \hat{n}_i n_{i+1}$$

with $h_x^{\text{sf}} = t$ and $U^{\text{sf}} = V$; we get $t_{i,i+1}^{\text{sf}} = t$ or t' and $V_{i,i+1}^{\text{sf}} = V$ or 0, respectively, for strong or weak bonds (i, i+1). Thus our spinfull chain includes the usual hopping and interaction a nearest-neighbor interaction and a field term along x in spin-space or a single-site spin-flip term. This kind of spin mapping will map spontaneous-current states to spin-current states with canted site-spin expectations, CDW to SDW, and BDW to an equivalent BDW/paramagnet as one may readily verify. The advantage of this kind of mapping is that we may carry known results from spinfull models to spinless models or vice versa.

Previously, the models of Refs. 36 and 37 are the best examples of spinfull ladders in the literature which exhibited spontaneous currents. Under Nersesyan's map, the model of Ref. 36 corresponds to a kind of tube spinless model *without* fourfold symmetry (which our tube model does have). Like us, they considered a strong-coupling limit in which the longitudinal hoppings were weakened; however, their path to spontaneous currents was unsatisfying from our viewpoint, in that it depended on a pair-hopping (ring exchange) term. Reference 37 exhibited a simpler spinfull ladder which was shown numerically to have currents; for a special choice of its parameters, Nersesyan's map takes that model to a spinless fermion tube model which does have fourfold symmetry. That mapped tube model still includes the same correlated hop of a diagonal pair as the Ref. 36 model.

V. TOWARD UNIFORM SPINLESS MODELS

Our hope was that if we can find a strong-coupling model that has spontaneous currents, perhaps it can be adiabatically continued to a translationally invariant model that does not distinguish the Hamiltonian terms on weak and strong plaquettes. There are two preconditions to even consider this: (i) the symmetry pattern of order should be consistent with a uniform order. Below, in Sec. V A, we verify this for our models. (ii) The "weak" and "strong" terms in the Hamil-



FIG. 5. The orbital current pattern in $|2+;2+\rangle$ state.

tonian should have the same form, differing only by the size of the coefficient. That is easy enough to manage, even if we adhere to the somewhat unnatural interaction term, Eq. (2.1b), with the nearest- and second-neighbor strengths made equal for convenience. If that equality is carried over to the interplaquette terms, it is actually beneficial since it cancels a term favoring CDW ordering [see Eq. (3.14)]

There is one further challenge: having conjectured a Hamiltonian favoring current ordering, how could we verify that? We need some family of variational wave functions that would (ideally) be definable for all the interpolating Hamiltonians from strong coupling to uniform and where the variational parameters allow any value of the spontaneous-current order parameter. (The best model of such a calculation is the recent work of Ref. 8.) In the case of the spinless ladder models, such a correspondence was already worked out by Nersesyan¹⁹ and is elaborated below in Sec. V B.

A. Interplaquette spontaneous currents

For the weak bonds, the required pseudocurrent operator is $\hat{I}_{weak} = i[c_{Ai}^{\dagger}c_{Bj} - c_{Bj}^{\dagger}c_{Ai}]$, where i-j is a weak bond. We again use the canonical transformation recipe, Eq. (A2) from the Appendix, but now for the purpose of deriving an expectation rather than a Hamiltonian term. The pseudocurrent operator for the weak bonds projects, in pseudospin language, to

$$\hat{I}_{weak} = -\frac{t'}{2(2t+V)} (|2+;2+\rangle\langle 2+;2+|-|2-;2-\rangle\langle 2-;2-|)$$
$$= -\frac{t'}{2(2t+V)} (P_A^z + P_B^z) = -\frac{t'}{2(2t+V)} (T_A^z - T_B^z). \quad (5.1)$$

Since the pseudospin operator for the strong bond is just $+\hat{P}^{z}/2$ [Eq. (2.5)], the weak-bond and strong-bond currents have *opposite* directions (Fig. 5), which is the same pattern as the *d*-density-wave (ddw) state.⁵ Thus, this pattern is consistent with a ddw-like state if we could analytically continue our model to a uniform one. For the tube lattice, the weak-bond currents are zero. That must be true to all orders on grounds of symmetry.

B. Uniform model

Can one of our strong-coupling models be connected to a uniform one, in which the distinction of strong and weak bond vanishes? We found the Nersesyan map (Sec. IV B) was the key to guessing a Hamiltonian that has a spontaneous-current ground state. The spinless model's pseudocurrent order maps (as we show shortly) to spincurrent order in the spinful model. One need only invent a *uniform* spin Hamiltonian giving the desired order and such that it maps to a plausible Hamiltonian of the spinless fermions. The only limitation is that the resulting spinless model is built from site pairs: it lends itself to ladders or bilayers, but not to (say) the fourfold symmetric square lattice.

The Nersesyan approach is an existence proof that if we get spontaneous-current order in a simple, local, strongcoupling model, the adiabatic extension can work all the way to the uniform case. If we could find an analogous starting point on the square lattice, that result would make the corresponding extension more plausible; unfortunately (Sec. V B) we could not find such a starting point.

Concerning the spin-current order mentioned above, consider a strong plaquette in our ladder with angular momentum +1 which has spontaneous pseudocurrents on its rungs and leg bonds. It maps to a pair of sites on the spinfull chain with Nersesyan spin expectations

$$\langle \tilde{S}_i \rangle \propto [1, (-1)^j, 0] \tag{5.2}$$

which corresponds correctly to a nonzero $\langle P_j^z \rangle = 1$ [see Eqs. (4.5) and (4.6)]. The uniform S_x component is not surprising, as every spinless ladder we consider includes a rung hopping which becomes an *x* transverse field under Nersesyan's map.

The pseudocurrent along a rung, I_i^{\perp} , maps to S_y , corresponding to the alternating y component. What about the pseudocurrents along the legs? Let us define a difference between the two sides,

$$I_i^{\parallel} \equiv I_{(i,1)\to(i+1,1)} - I_{(i,2)\to(i+1,2)}.$$
(5.3)

Of course, in the expected state, opposite sides have opposite currents, so this also has a nonzero expectation. Evidently, this simply maps to the *z* component of *spin current* from $i \rightarrow i+1$, $I_{i\rightarrow i+1}^{S}$. Indeed, in spin models with an isotropic Hamiltonian (and also here), spin current goes with the twist between noncollinear spins, $\vec{I}_{i\rightarrow j} \propto \mathbf{S}_i \times \mathbf{S}_j$ and indeed, the staggering of rung-spin directions in Eq. (5.2) does give the requisite nonzero (and alternating) $(\mathbf{S}_i \times \mathbf{S}_{i+1})_z$ component.

Now we see a simple route to a *uniform* model having spontaneous currents: simply find a uniform Hamiltonian for a spin-1/2 chain, having a ground state with the above staggered spin canting. The simplest realization (from the spin chain viewpoint) would be an antiferromagnetic chain with (i) an S_x field, so the spins will cant transverse to it plus (ii) a small anisotropy in the antiferromagnetic exchange, such that the S_y axis is easier than S_z ; this ensures the canting happens in the *y* direction. The problem with following this route literally is ingredient (ii): S_x - S_x or S_y - S_y spin couplings correspond, in the spinless model, to two-fermion pair correlated hops in a plaquette, which we did not want to include. Conversely, this illustrates why correlated hopping is conducive to the existence of spontaneous currents.⁴

The scenario of the previous paragraph can be achieved, instead, with the following adjustment of the Hamiltonian: in place of a spin chain, take a *Hubbard* chain with a transverse x field h_x^{sf} , as above, plus a small *ferromagnetic* coupling J_z^{sf} of neighboring S^z components. A strong Hubbard on-site repulsion U^{sf} provides the effective antiferromagnet exchange

at order $(t^{sf})^2/U^{sf}$, in the standard fashion. Via the Nersesyan map [see Eqs. (4.5) and (4.6)], we realize that: (1) the transverse field suppressing spin ordering in *x* direction maps to a term suppressing of BDW in the spinless ladder, (2) the small ferromagnetic *z* coupling suppressing spin ordering in *z* direction (by reducing the strength of *z* antiferromagnetic exchange) maps to a term suppressing CDW in the spinless ladder, and finally (3) due to the aforesaid suppressions, stabilization of spin order in the *y* component maps to orbital currents for the spinless ladder.

In the spinless language, the Hubbard U^{sf} and $-J_z^{\text{sf}}S_i^z S_{i+1}^z$ interactions just map, respectively, to nearest-neighbor interactions along the rungs and legs (repulsive V_{\perp} and attractive V_{\parallel}). The Hubbard hopping t^{sf} and the transverse field h_x^{sf} just map, respectively, to hoppings along the rungs and legs (our t_{\perp} and t_{\parallel}). The half filling we adopted for the spinless model corresponds to half filling in the Hubbard model. Unlike all spinless models we previously mentioned, this model is a uniform ladder with *no weak and strong plaquettes*.

The above paragraph is essentially a rediscovery of Nersesyan's ladder model, Eq. (1) of Ref. 19. In particular, our key ingredient, making V_{\parallel} attractive while V_{\perp} repulsive and zero $V_{\sqrt{2}}$, is essentially the same as Nersesyan's recipe, which is that $V_{\sqrt{2}}-V_{\parallel}>0$. It is interesting to note these chains have fractionalized excitations, domain walls carrying 1/2 fermion charge,²⁰ corresponding to spinons in the spin model.

Extension to the square lattice?

The same mapping can be used in one dimension higher, to build a spinless spontaneous-current state on a bilayer from a Hubbard model on a square lattice²¹ (or any bipartite lattice). A *spinfull* model with plausible interactions on that same lattice was known earlier³⁸ that exhibits spontaneous currents. That model's Hamiltonian is similar to the Scholl-wöck *et al.*³⁷ ladder in one dimension higher and is similarly engineered to have an SO(5) symmetric point. (A minor difference is their interlayer hopping may differ from the inlayer hopping.) All their interaction terms and (isotropic) exchange act only on rungs. Thus, the main qualitative difference between our model (apart from spin, of course) would be our inlayer repulsion term. The (conjectured) order in our bilayer model is the same alternating pattern of currents as in their model (Fig. 1 of Ref. 38).

Unfortunately, this does not work for the plain square lattice, for two reasons.³⁹ First, the best we could manage for a Hamiltonian (Sec. III E 3) depended on t''_3 and $t''_{\sqrt{10}}$ hoppings to a second neighbor plaquette while the much shorter hoppings entering Eq. (3.18b) must be negligible. Not only are those absurdly distant neighbors to have a meaningful hopping: once we make the lattice uniform, we must also include t'_3 and $t'_{\sqrt{10}}$ of the same separations as t''_3 and $t''_{\sqrt{10}}$ but coupling *nearest*-neighbor plaquettes and creating the undesired unfrustrated anisotropy, Eq. (3.18b). Second, we cannot be guided by Nersesyan's map, as it demands that sites come in *pairs*.

Although, it seems difficult to obtain currents order in a uniform square lattice, the terms which worked in the ladder would still be effective in a rectangular lattice. That suggests one possibility to obtain spontaneous currents as a symmetry breaking. Notice that a *uniform* bond order, i.e., the state currently called electron nematic²⁵ reduces the system to rectangular symmetry, making $t_{\parallel} \neq t_{\perp}$ heuristically [see Sec. III C 2). Thus, spontaneous currents could be parasitic on electron nematic order. This is a not a linear coupling of the two order parameters; it would be a second Ising-type transition, to a state breaking $Z_2 \times Z_2$ symmetry.

VI. DISCUSSION

The central aim of this paper was to investigate the possibilities of a lattice model *manifestly* displaying spontaneous currents in its ground state. Among our models, containing standard hopping and interaction terms, it was fairly difficult to stabilize only the spontaneous-current state. Frequently, there was a remnant continuous symmetry leading to an arbitrary mixing with one of the competing orders; and most perturbations which could break that degeneracy tended to favor the competing order. Something similar also happens in some spinfull models meant to address the possibility of spontaneous currents in a realistic system, e.g., the relation²⁶ of *d*-density-wave current order and electron-nematic order (related to our bond order).

We did show that rather contrived and unappealing fermion interaction or hopping terms could be used to stabilize currents but it seems highly unlikely that those kinds of processes are at work in real materials. We suggest our finding may be related to the rarity of solids in nature having spontaneous currents in their ground state.³⁹

A. Summary

The central results of this paper are as follows. We emphasize first that our microscopic Hamiltonian was limited to (mainly spinless) models with interactions and one-fermion hopping terms. We did not explore the possibilities of correlated hopping, which were already known to be conducive to the *d*-density-wave current order.^{4,36} Ultimately such terms come microscopically from higher-order processes in fermion hops; thus, within our picture, related terms might be accessed by expanding our canonical transformation (Sec. III and Appendix) to higher orders, producing effective interactions with higher powers of pseudospin.

We showed that by tuning the parameters and the underlying geometry of a toy spinless Hamiltonian, we can make a system acquire spontaneous currents, charge or bond order. The crucial ingredient of our analysis was the pseudospin mapping (Sec. II B) and degenerate second-order perturbation theory (Appendix). We saw that bond ordering is naturally disfavored in ladders (Sec. III B); while, for tube and square lattice, the ground state can acquire possibly coexisting charge, bond or current order in a symmetry breaking fashion (Secs. III A and III B). Since, the tube is quasi one dimensional, the correlation will actually be power laws; but for the square lattice, we will have true long-range order. Furthermore, the pattern of currents corresponding to the spontaneous currents carrying ground state is same as the d-density-wave state (Sec. V A). The Nersesyan map provided a way to extend our strong-coupling result to that of an uniform case for the ladder (Sec. V B).

B. Relation to three-band model and other real systems

The current contact of our topic with real systems is in the three-band model of cuprates.^{3,15} A recent paper⁷ argued (by mapping to a two-channel Luttinger liquid and then analytic perturbation) that a ladder version of the three-band model of cuprates has long-range order with a current pattern similar to Varma's state. This claim was brought into question by a subsequent density matrix renormalization group (DMRG) calculation⁴⁰ on the same model: the current-current correlations were seen (numerically) to decay with a power law. But that, of course, indicates the presence of gapless excitations, such as the Goldstone mode of a continuous symmetry; it would *not* expected for the Ising-type symmetry of a (pseudo)current operator, unless the system is accidentally at a critical point.

In our spinless model, it was easy enough to get current order degenerate with bond-density order or to stabilize the latter, but quite hard to stabilize just current order. Could this be going in the ladder system of Refs. 7 and 40 in which the current operator is just one component of a larger order parameter with XY symmetry? We warn, however, that our results also suggest that ladders (applied as an approach to square lattice models³⁷) are plain deceptive. The key terms stabilizing currents depended on the very anisotropy of the ladder.

For that reason, it is interesting that Ref. 8 do claim to obtain currents in a variational and truly two-dimensional calculation. So far, there is no clear picture of which interactions are crucial to causing the order. A strong-coupling caricature of the three-band lattice (or ladder) in the spirit of our models might illuminate this point.

ACKNOWLEDGMENTS

C.L.H. thanks S.-A. Cheong, D. I. Khomski, U. Hizi, M. Troyer, G. Kotliar, and J. B. Marston for discussions. This work was supported by NSF under Grant No. DMR-0552461.

APPENDIX: CANONICAL TRANSFORMATION

Since we use the method of canonical transformation for our calculations, here is a very brief summary of the method and the results that are used. Say that \mathcal{H}^0 represents the strong-coupling limit, which is assumed to have eigenenergies $\{E_{\alpha}\}$ with a large ground-state degeneracy, which however is split by a small perturbation \mathcal{H}' (that has no matrix elements between degenerate states of \mathcal{H}^0). We desire to project our problem onto the ground-state ("zero") subspace of \mathcal{H}^0 . The usual way to accomplish this is canonical transformation: let $\tilde{\mathcal{H}} \equiv e^{iS} \mathcal{H} e^{-iS}$, where we require $\tilde{\mathcal{H}}_{\alpha\beta} = 0$ for any matrix element connecting the zero subspace to other states; then, we can restrict our Hilbert space to the span of $e^{iS} |\alpha\rangle$, where $|\alpha\rangle$ was one of the ground states.

To lowest order in \mathcal{H}' , the standard canonical transformation is given by $S_{\alpha\beta} \equiv 0$ when states α and β are degenerate, and $S_{\alpha\beta} \equiv i\mathcal{H}'_{\alpha\beta}/(E_{\beta}-E_{\alpha})$ otherwise. Then the effective Hamiltonian is given by $\widetilde{\mathcal{H}} = \mathcal{H} + \delta \mathcal{H}$, where SUMIRAN PUJARI AND C. L. HENLEY

$$\delta \mathcal{H}_{\alpha\beta} \equiv -\frac{1}{2} \sum_{\gamma} \left(\frac{1}{E_{\gamma} - E_{\alpha}} + \frac{1}{E_{\gamma} - E_{\beta}} \right) \mathcal{H}_{\alpha\gamma}' \mathcal{H}_{\gamma\beta}' \quad (A1)$$

is the *off-diagonal* second-order perturbation correction. Similarly, an operator \mathcal{O} is transformed to $\widetilde{\mathcal{O}} = \mathcal{O} + \delta \mathcal{O}$, where (to lowest order)

$$\delta \mathcal{O}_{\alpha\beta} \equiv i \sum_{\lambda} \left(\frac{\mathcal{H}'_{\alpha\lambda} \mathcal{O}_{\lambda\beta}}{E_{\lambda} - E_{\alpha}} - \frac{\mathcal{O}_{\alpha\lambda} \mathcal{H}'_{\lambda\gamma}}{E_{\lambda} - E_{\beta}} \right).$$
(A2)

For our problem, $\mathcal{H}^{hop} + \mathcal{H}^{V}$ is the strong-coupling limit and \mathcal{H}' is the small perturbation.

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