Tuning Kinetic Magnetism of Strongly Correlated Electrons via Staggered Flux

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We explore the kinetic magnetism of the infinite-U repulsive Hubbard models at low hole densities on various lattices with nearest-neighbor hopping integrals modulated by a staggered magnetic flux $\pm \phi$. Tuning $\phi$ from $0$ to $\pi$ makes the ground state (GS) change from a Nagaoka-type ferromagnetic state to a Haerter-Shastry-type antiferromagnetic state at a critical $\phi_c$, with both states being of kinetic origin. Intra-plaquette spin correlation, as well as the GS energy, signals such a quantum criticality. This tunable kinetic magnetism is generic, and appears in chains, ladders and two-dimensional lattices with squares or triangles as elementary constituents.

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Introduction.—The study of magnetism may begin with a Heisenberg-type model in which localized spins interact with each other. However, the fundamental interaction between electrons is the Coulomb-like repulsion, while the Pauli principle could induce a spin dependence when electrons are not localized. The Nagaoka theorem provides us a rigorous mechanism that the saturated ferromagnetic (FM) state of kinetic origin is the unique ground state (GS) when a single hole is inserted into the half-filled Hubbard model with an infinite on-site repulsion $U$. In the Nagaoka’s problem, the sign of the hopping amplitudes around the smallest closed loop in a lattice, $S_{\text{loop}}$, is necessarily positive.

In a recent letter, Haerter and Shastry (HS) have made important progress in an opposite situation to Nagaoka’s problem, a single hole moving in the infinite-$U$ Hubbard model on two-dimensional (2D) triangular lattices with frustrated hopping, i.e., $S_{\text{loop}}$ of an elementary triangle is negative [2]. Through numerical exact diagonalization (ED) studies of finite lattices, they found that the motion of a single hole with the electronic frustration leads to weak metallic antiferromagnetism (AF) of kinetic origin.

There are still two important issues to be resolved. One is whether there is a tunable transition between the two opposite kinetic magnetisms. The other is whether or not the two kinetic magnetisms can appear in the systems with more holes or with finite hole densities, which are much closer to experimental realities. Therefore, we are motivated to study the infinite-$U$ Hubbard models at low hole densities on various lattices with nearest-neighbor hopping integrals modulated by a staggered magnetic flux $\pm \phi$. In these systems, $S_{\text{loop}} = \exp(i\phi)$ can be tuned from $+1$ to $-1$ via the Aharonov-Bohm effect, $\phi = 0$ and $\phi = \pi$ correspond respectively to Nagaoka’s and HS’s problems, and the spatial periodicity is preserved when $\phi$ varies from $0$ to $\pi$.

Our motivations also come from three other aspects: our problem is relevant to future experiments applying an external magnetic field on artificial lattices of quantum dots [3] or creating an artificial magnetic field on optical lattices of ultracold fermionic atoms [4]; an effective magnetic flux can be induced intrinsically through some mechanisms in strongly correlated systems [3, 5]; and our problem presents a concrete example to study quantum phase transitions in both finite and infinite systems [5] with a tunable parameter $\phi$.

On the basis of ED calculations of finite systems and analytical estimations of infinite systems, we find that tuning $\phi$ from $0$ to $\pi$ makes the GS change from a Nagaoka-type FM state to an HS-type AF state at a critical $\phi_c$. Intra-plaquette spin correlation, as well as the GS energy, signals such a quantum criticality. This tunable kinetic magnetism is generic, and appears in many lattice structures with squares or triangles as elementary constituents: elementary square and triangle, diamond and sawtooth chains, square and trestle ladders, 2D square and triangular lattices.
The infinite-U Hubbard model

Model Hamiltonian. The infinite-U Hubbard model with a staggered flux (SF) can be written as:

\[ H = t \sum_{\langle ij \rangle} \epsilon^{\pi s_{ij}} (1 - n_{j,-\sigma}) c_{j,-\sigma}^\dagger c_{i,\sigma} (1 - n_{i,-\sigma}) + \text{H.c.} \]  

where the hopping integral \( t \) is positive and is taken as the unit of energy, \( c_{i,\sigma} (c_{i,\sigma}^\dagger) \) is an electron annihilation (creation) operator on site \( i \) of spin \( \sigma = \uparrow \) or \( \downarrow \), \( n_{i,\sigma} \) is the electron number operator, and \( \langle ij \rangle \) refers to two nearest neighboring sites. The magnetic flux per plaquette (the summation of \( a_{ij} \) along four links around a plaquette) is given by \( \pm \phi \) alternatively in neighboring plaquettes, with \( \phi \) in units of \( \phi_0 = 2\pi \pi/e \) (the flux quantum). Since the system is symmetric under the transformations \( \phi \rightarrow -\phi \) and \( \phi \rightarrow 2\pi - \phi \), it is sufficient to restrict \( \phi \) to the interval \([0, \pi]\). The hole number is \( N_h = N_L - N_e \), where \( N_L \) and \( N_e \) are the numbers of sites and electrons, respectively; the hole density is denoted by \( x = N_h/N_L \).

The symmetric gauge is chosen for this SF as shown in Fig. 1 and the corresponding periodical boundary conditions are adopted. It should be noted that translational and macroscopic time-reversal symmetries make our model distinct from the uniform flux case, where the energy spectrum exhibits the fractal Hofstadter butterfly and the uniform flux induces a saturated FM from statistical transmutation at a flux quantum per electron [3].

Toy models of elementary square and triangle. As an illustration of basic physics, we first consider toy models of elementary square and triangle with a single hole \( (N_h = 1) \) which can be solved analytically. For the elementary square, when \( \phi \) increases from 0 to \( \pi \), at \( \phi_c = \pi/3 \), the GS transits from a state with the maximum total spin \( S_{\text{tot}} = \frac{3}{2} \) (a Nagaoka FM) to a state with \( S_{\text{tot}} = \frac{3}{2} \), and the nearest-neighbor (n.n.) spin correlation changes from \( \frac{1}{8} \) to \( -\frac{1}{8} \). For the elementary triangle, when \( \phi \) increases from 0 to \( \pi \), at \( \phi_c = \pi/2 \), the GS transits from a \( S_{\text{tot}} = 1 \) state to a \( S_{\text{tot}} = 0 \) state, and the n.n. spin correlation changes from \( \frac{1}{12} \) to \( -\frac{1}{12} \).

Diamond and sawtooth chains. On a periodic lattice with an SF, the lowest kinetic energy of a single hole in a saturated FM spin background, \( E_{\text{FM}}^{1\text{h}}(\phi) \), can be obtained via the Fourier transformation. For an infinite diamond chain, \( E_{\text{FM}}^{1\text{h}}(\phi) = -2\sqrt{2}\cos(\phi/4) \); while for a sawtooth chain, \( E_{\text{FM}}^{1\text{h}}(\phi) = -(1 + \sqrt{6}) \cos(\phi/3) \).

FIG. 2: (color online). (a), (b) Diamond chains. (c), (d) Sawtooth chains. \( m \)'s and rescaled GS energies versus \( \phi \) in the cases with various sizes and hole numbers. We will present typical ED data obtained by using the Spinpack package [3] and exploiting the translational invariance in the subspace with fixed \( S_{\text{tot}} \) (0 for even \( N_e \), and \( \frac{1}{4} \) for odd \( N_e \)). The commonly used quantity in evaluating Nagaoka FM, i.e. the GS \( S_{\text{tot}} \), is strongly dependent upon the boundary conditions chosen and the even/odd parity of \( N_h \) [8, 11, 12]. We therefore concentrate on two derived quantities which are not sensitive to the boundary condition or the parity of \( N_h \).

The first quantity, \( m \), is used to measure the spin correlations intra a plaquette. For a square plaquette, \( m_1 = \frac{1}{4} + \langle S_2 \cdot S_3 \rangle + \langle S_2 \cdot S_4 \rangle + \langle S_3 \cdot S_4 \rangle \) (with four clockwise sites 1, 2, 3 and 4, and \( \langle \cdot \cdot \cdot \rangle \) means the GS average) [13], and the average over four sites gives \( m_\square = \frac{1}{4} \sum_{i=1}^{4} m_i \). On the square lattice, \( m_\square = 1 \) in a classical FM state, \( m_\square = 0 \) in a classical Néel AF state, while \( m_\square = \frac{1}{4} \) if there is no spin correlation. For a triangular plaquette, \( m_1 = \frac{1}{2} + \langle S_2 \cdot S_3 \rangle \), and the average over three sites gives \( m_\triangle = \frac{1}{3} \sum_{i=1}^{3} m_i \). On the triangular lattice, \( m_\triangle = 1 \) in a classical FM state, \( m_\triangle = \frac{1}{3} \) in a classical 3-sublattice 120° AF state, while \( m_\triangle = \frac{1}{6} \) if there is no spin correlation. The other quantity, the rescaled GS energy \( E(\phi)/|E(0)| \), is used to compare the non-analyticities in GS energies of various cases.

For the 12-site and 18-site diamond chains with respectively \( N_h = 1 - 2 \) and \( N_h = 1 - 4 \), when \( \phi \) changes from 0 to \( \pi \), \( m_\square \)'s drop almost abruptly near a \( \phi_c \approx \pi/3 \) [Fig. 2(a)]. (Note that \( \phi_c = \pi/3 \) for the elementary square with \( N_h = 1 \).) Meanwhile, the GS energies also show clearly certain non-analyticities near \( \pi/3 \) [Fig. 2(b)].

For the 12-site and 18-site sawtooth chains with respectively \( N_h = 1 - 3 \) and \( N_h = 1 - 4 \), as seen from

| Elementary Square | \( S_{\text{tot}} \) of GS \( \langle S_i \cdot S_j \rangle_{\text{n.n.}} \) | GS Energy |
|-------------------|-----------------|-------------|
| \( 0 \leq \phi < \pi/3 \) | 3/2 | \( 1/8 \) | \( -2\cos(\phi/4) \) |
| \( \pi/3 < \phi < \pi \) | 1/2 | \( -1/8 \) | \( -2\cos(\phi/4 - \pi/6) \) |

| Elementary Triangle |
|---------------------|
| \( 0 \leq \phi < \pi/2 \) | 1 | \( 1/12 \) | \( -2\cos(\phi/3) \) |
| \( \pi/2 < \phi < \pi \) | 0 | \( -1/4 \) | \( -2\cos(\phi/3 - \pi/3) \) |
Figs. 2(c) and (d), the abrupt drops of \( m_{\Delta} \)'s and non-analyticities in GS energies occur near a \( \phi_c \approx \pi/2 \). (Note that \( \phi_c = \pi/2 \) for the elementary triangle with \( N_h = 1 \).

In the four cases of diamond chains \( (N_L = 12 \text{ with } N_h = 1, N_L = 18 \text{ with } N_h = 1-3) \) and all seven cases of sawtooth chains, \( m \)'s change very little (and the systems possess intra-plaquette FM correlations since all \( m \)'s satisfy \( m > \frac{1}{2} \)) when \( \phi \) varies from 0 to \( \phi_c \), and the curves of rescaled GS energies are very close to that of \( E_{1h}^{FM}(\phi)/|E_{FM}^{BR}(0)| \) [the continuous curves in Figs. 2(b) and (d)]. (The ED data also tell us that in each case with odd \( N_h \), the GS \( S_{\text{tot}} \) takes the maximum value \( N_c/2 \) when \( 0 \leq \phi \ll \phi_c \).) Since \( \phi = 0 \) corresponds to the Nagaoka FM \( (S_{\text{loop}} = +1) \) and \( m \)'s change little for \( 0 \leq \phi < \phi_c \), we extend the notion of Nagaoka FM here and such a state (with \( \phi_c < \phi \leq \pi \)) is referred to as a Nagaoka-type AF.

**Square and trestle ladders.**—For the single-hole Nagaoka FM in an infinite square ladder with an SF, \( E_{1h}^{FM}(\phi) = -\sqrt{5 + 4 \cos(\phi/2)} \); while in an infinite trestle ladder, \( E_{1h}^{FM}(\phi) = -4 \cos(\phi/3) \).

For the \( 8 \times 2, 10 \times 2 \) and \( 12 \times 2 \) square ladders with respectively \( N_h = 1-3, N_h = 2-4 \) and \( N_h = 1-2 \), as seen from Figs. 3(a) and (b), the abrupt drops of \( m_{\Delta} \)'s and non-analyticities in GS energies occur near different \( \phi_c \)'s, with \( \phi_c \) versus hole density \( x \) varying rather smoothly.

For the \( 6 \times 2 \) and \( 9 \times 2 \) trestle ladders with respectively \( N_h = 1-3 \) and \( N_h = 1-4 \) [Figs. 3(c) and (d)], the abrupt drops of \( m_{\Delta} \)'s and non-analyticities in GS energies also occur near different \( \phi_c \)'s, with still a smooth curve of \( \phi_c \) versus \( x \).

In these cases of square and trestle ladders, \( m \)'s change very little and satisfy \( m > \frac{1}{2} \) when \( \phi \) varies from 0 to \( \phi_c \), the curves of rescaled GS energy are very close to that of \( E_{1h}^{FM}(\phi)/|E_{FM}^{BR}(0)| \), and these states are of Nagaoka-type FMs; when \( \phi \) varies from \( \phi_c \) to \( \pi \), all \( m \)'s show obvious intra-plaquette AF correlations, and these states are of HS-type AFs.

It is tempting to estimate \( \phi_c \) in the limit of low hole density \( (x \to 0) \). Such a task can be partly fulfilled with the Brinkman-Rice (BR) approximation [14]. For a single hole in an infinite Néel AF spin background, the BR approximation accounts the dominant contributions to the self energy of single-hole Green’s function, i.e., the retracetable paths without any closed loop. Such an approximation leads to a hole band edge (i.e., the lowest single-hole kinetic energy) \( E_{AF}^{BR} = -2\sqrt{z-1} \), where \( z \) is the coordination number.

Through comparison between \( E_{AF}^{BR} \) and \( E_{1h}^{FM}(\phi) \) of a single hole in infinite ladders, one can obtain a rough estimation of \( \phi_c \) in the limit \( x \to 0 \). For an infinite square ladder, \( z = 3 \), and \( E_{AF}^{BR} = E_{1h}^{FM}(\phi) \) gives a \( \phi_c^{BR} = 2 \arccos(3/4) \approx 0.46\pi \). For an infinite trestle ladder, \( z = 4 \), and \( E_{AF}^{BR} = E_{1h}^{FM}(\phi) \) gives a \( \phi_c^{BR} = \pi/2 \).

**Square and triangular lattices.**—For the single-hole Nagaoka FM in an infinite square lattice with an SF, \( E_{FM}^{BR}(\phi) = -4 \cos(\phi/4) \); while for an infinite triangular lattice, \( E_{FM}^{BR}(\phi) = -6 \cos(\phi/3) \).

For the \( 4 \times 4 \) and \( 6 \times 4 \) square lattices with respectively \( N_h = 1-4 \) and \( N_h = 1-2 \) [Figs. 3(a) and (b)], or the \( 3 \times 3 \) and \( 6 \times 3 \) triangular lattices with respectively \( N_h = 1 \) and \( N_h = 1-3 \) [Figs. 3(c) and (d)], the abrupt drops of \( m \)'s and non-analyticities (or changes of concavities) in GS energies also occur near different \( \phi_c \)'s. In all these cases, the GSs are of Nagaoka-type FMs for \( 0 \leq \phi < \phi_c \), and are of HS-type AFs for \( \phi_c \ll \phi \leq \pi \). The curve of \( \phi_c \) vs. \( x \) of the square lattices [the inset in Fig. 3(b)] approaches a critical doping \( x_c \sim 0.3 \) at \( \phi_c = 0 \), which agrees well with the quantum Monte Carlo studies on the instability of saturated Nagaoka FM against doping [12].

A rough estimation of \( \phi_c \) in the limit \( x \to 0 \) with the aid of the BR approximation is: \( \phi_c^{BR} = 2\pi/3 \) for an infinite square lattice, and \( \phi_c^{BR} = 3 \arccos(\sqrt{5}/3) \approx 0.70\pi \) for an infinite triangular lattice.

**Long-range spin correlations and ordering.**—As seen from the above, the two quantities, \( m \) and \( E(\phi)/|E(0)| \), describe well the transitions from the Nagaoka-type FM to the HS-type AF. The ED data of the six kinds of lattices also tell us that for each case with odd \( N_h \), the GS \( S_{\text{tot}} \) always takes the maximum value \( N_c/2 \) and \( (S_{\text{tot}})^+ \) is positive and almost a constant for any range \( r \) when

FIG. 3: (color online). (a),(b) Square ladders. (c),(d) Trestle ladders. \( m \)'s and rescaled GS energies versus \( \phi \) in the cases with various sizes and hole numbers. The insets in (b) and (d) show \( \phi_c \) vs. hole density \( x \).
0 ≤ φ ≪ φ_c, namely, the Naogoka-type states are long-range ordered FM. Now we would take a closer look at the long-range spin correlations of the cases with even \( N_h \)'s. We focus on the three cases of square ladders (in which there are the longest-range spin correlations) as examples: \( N_L = 10 \times 2 \) and \( N_h = 2, 4, N_L = 12 \times 2 \) and \( N_h = 2 \).

In an artificial lattice of quantum dots, a large lattice constant would enable us to observe this effect at a modest flux strength of a few Tesla [3]. This effect could also be realized in optical lattices of ultracold atoms if appropriate phase factors are introduced for hopping integrals by laser assisted hopping, lattice tilting and other experimentally accessible techniques [4].

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