Tuning Kinetic Magnetism of Strongly Correlated Electrons via a Staggered Flux

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An interplay between kinetic process and magnetic ordering is manifested when strong correlation and electronic frustration are present: tuning a staggered flux ϕ from 0 to π makes the ground state (GS) of an infinite-U Hubbard model change abruptly from a Nagaoka-type ferromagnet to a Haerter-Shastry-type antiferromagnet at a ϕ_c, with both states being metallic and of kinetic origin. Intraplaquette spin correlation, as well as nonanalyticity in the GS energy, signals such a novel quantum criticality. This tunable kinetic magnetism is generic and may be experimentally realized.

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Introduction.—Understanding the magnetic behavior of metallic compounds is a challenging problem. The Nagaoka theorem provides us a rigorous mechanism that the metallic saturated ferromagnetic (FM) state of kinetic origin is the unique ground state (GS) when a single hole is inserted into the half-filled infinite-U repulsive Hubbard model [1]. In the Nagaoka's problem, the sign of the hopping amplitudes around the smallest closed loop in a lattice, $\mathcal{S}_{\text{loop}}$, necessarily takes the value $+1$. Recently, Haerter and Shastry (HS) have made important progress in an opposite situation, and have found that the motion of a single hole with the electronic frustration ($\mathcal{S}_{\text{loop}} = -1$) leads to weak metallic antiferromagnetism (AFM) of kinetic origin [2]. The HS mechanism plays a key role in explaining the newly found mysterious Curie-Weiss metallic phase in cobalt oxide systems [3].

An interesting question arises: what is the physics of a strongly correlated system between the two extreme situations of $\mathcal{S}_{\text{loop}} = +1$ (no frustration) and $\mathcal{S}_{\text{loop}} = -1$ (maximum frustration). Recent experimental advances provide possible techniques for tuning $\mathcal{S}_{\text{loop}}$ in various systems: applying an external magnetic field on artificial planar lattice of quantum dots [4–6] or a periodic net of carbon nanotubes connected by point tunneling contacts [7]; creating an effective magnetic field on optical lattices of ultracold fermionic atoms [8]; an effective magnetic flux induced intrinsically in pyrochlore-structure compounds [9]; a superconducting wire network decorated with an array of mesoscopic ferromagnets [10].

We are motivated to investigate 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, $\mathcal{S}_{\text{loop}} = \exp(i\phi)$ 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 ϕ varies from 0 to π. Based on exact diagonalization (ED) calculations and analytical estimations, we have found a generic behavior: tuning ϕ from 0 to π makes the GS change abruptly from a Nagaoka-type FM state to an HS-type AFM state at a critical ϕ_c; intraplaquette spin correlation, as well as nonanalyticity in the GS energy, signals such a novel quantum criticality.

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

$$H = t\sum_{\langle ij\rangle\sigma} e^{ia_{ij}}(1 - n_{j,-\sigma})c^{\dagger}_{j\sigma}c_{i\sigma}(1 - n_{i,-\sigma}) + \text{H.c.} \quad (1)$$

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

The symmetric gauge is shown in Fig. 1, and periodical boundary conditions are adopted. It should be noted that our model is distinct from the uniform flux case, where the energy spectrum exhibits the fractal Hofstadter butterfly and a saturated FM from statistical transmutation is induced at a flux quantum per electron [11].

Toy models of elementary square and triangle.—As an illustration, we first consider elementary square and triangle with a single hole ($N_h = 1$) which can be solved analytically (Table I). For the elementary square, when ϕ increases from 0 to π, 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 $S_{\text{tot}} = \frac{1}{2}$ state, and the nearest-neighbor (NN) spin correlation changes from $\frac{1}{8}$ to $-\frac{1}{8}$. For $0 < \phi < \pi/3$, the first excited state has $S_{\text{tot}} = \frac{1}{2}$, $\langle S_i \cdot S_j\rangle_{\text{NN}} = -\frac{1}{8}$ and energy $E = -2\cos(\phi/4 - \pi/6)$; for $\pi/3 < \phi < 2\pi/3$, the

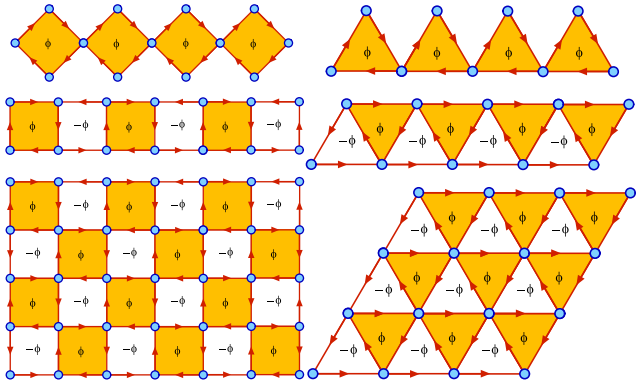

FIG. 1 (color online). Left: Diamond chain, square ladder and 2D square lattice. Right: Sawtooth chain, trestle ladder and 2D triangular lattice. Each arrow represents a phase shift.

first excited state has $S_{\rm tot}=\frac{3}{2}$, $\langle S_i\cdot S_j\rangle_{\rm NN}=\frac{1}{8}$ and $E=-2\cos(\phi/4)$; while for $2\pi/3<\phi<\pi$, the first excited state has $S_{\rm tot}=\frac{1}{2}$, $\langle S_i\cdot S_j\rangle_{\rm NN}=-\frac{1}{8}$ and $E=-2\cos(\phi/4-\pi/3)$. For the elementary triangle, when ϕ increases from 0 to π, at $\phi_c=\pi/2$, the GS transits from a $S_{\rm tot}=1$ state to a $S_{\rm tot}=0$ state, and the NN spin correlation changes from $\frac{1}{12}$ to $-\frac{1}{4}$. Such results should shed new light on experiments with four or three self-assembled quantum dots [5,6].

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, $E^{\rm 1h}_{\rm FM}(\phi)$, can be obtained via the Fourier transformation. For an infinite diamond chain, $E^{\rm 1h}_{\rm FM}(\phi)=-2\sqrt{2}\cos(\phi/4)$; while for a sawtooth chain, $E^{\rm 1h}_{\rm FM}(\phi)=-(1+\sqrt{5})\cos(\phi/3)$.

We will present typical ED data obtained by using the Spinpack package [12] for the subspace with fixed $S^z_{\rm tot}$ (0 for even N_e, and $\frac{1}{2}$ for odd N_e). The commonly used quantity in evaluating Nagaoka FM, i.e., the GS $S_{\rm tot}$, is strongly dependent upon the boundary conditions chosen and the even or odd parity of N_h [11,13–15]. We therefore concentrate on two derived quantities which are not sensitive to the boundary conditions or the parity of N_h.

The first quantity, m, is used to measure the intraplaquette spin correlations. For a square plaquette, $m_1\equiv\frac{1}{4}+\langle S_2\cdot S_3\rangle+\langle S_2\cdot S_4\rangle+\langle S_3\cdot S_4\rangle$ (with four clockwise sites 1, 2, 3 and 4, and $\langle\ldots\rangle$ means the GS average) [16], 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 AFM state, while $m_\square=\frac{1}{4}$ if there is no spin correlation. For a triangular plaquette, $m_1\equiv\frac{1}{2}+2\langle S_2\cdot S_3\rangle$, 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, $m_\triangle=\frac{1}{4}$ in a classical 3-sublattice 120° AFM state, while $m_\triangle=\frac{1}{2}$ if there is no spin correlation. The other quantity, the rescaled GS energy $E(\phi)/|E(0)|$, is used to compare the nonanalyticities in GS energies of various cases.

TABLE I. Elementary square and triangle: GS properties of the cases with $N_h=1$.

	Elementary square		
ϕ	$S_{\rm tot}$ of GS	$\langle S_i\cdot S_j\rangle_{\rm NN}$	GS energy
$0\le\phi<\pi/3$	3/2	1/8	$-2\cos(\phi/4)$
$\pi/3<\phi<\pi$	1/2	−1/8	$-2\cos(\phi/4-\pi/6)$
	Elementary triangle		
ϕ	$S_{\rm tot}$ of GS	$\langle S_i\cdot S_j\rangle_{\rm NN}$	GS energy
$0\le\phi<\pi/2$	1	1/12	$-2\cos(\phi/3)$
$\pi/2<\phi\le\pi$	0	−1/4	$-2\cos(\phi/3-\pi/3)$

For the 12-site and 18-site diamond chains with, respectively, $N_h=1$–2 and $N_h=1$–4, when ϕ changes from 0 to π, $m_\square$'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 nonanalyticities 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 Figs. 2(c) and 2(d), the abrupt drops of $m_\triangle$'s and nonanalyticities 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 ($N_L=12$ with $N_h=1$, $N_L=18$ with $N_h=1$–3) and all seven cases of sawtooth chains, m's change very little (and the systems possess intraplaquette FM correlations since all m's satisfy $m>\frac{1}{2}$) when ϕ varies from 0 to ϕ_c, and the curves of rescaled GS energies are very close to that of $E^{\rm 1h}_{\rm FM}(\phi)/|E^{\rm 1h}_{\rm FM}(0)|$ [the continuous curves in Figs. 2(b) and 2(d)]. (The ED data also tell us that in each case with odd N_h, the GS $S_{\rm tot}$ takes the maximum value $N_e/2$ when $0\le\phi\ll\phi_c$.) Since $\phi=0$ corresponds to the Nagaoka FM ($\mathcal{S}_{\rm loop}=+1$) and m's change little for $0\le\phi<\phi_c$, we extend the notion of Nagaoka FM here and

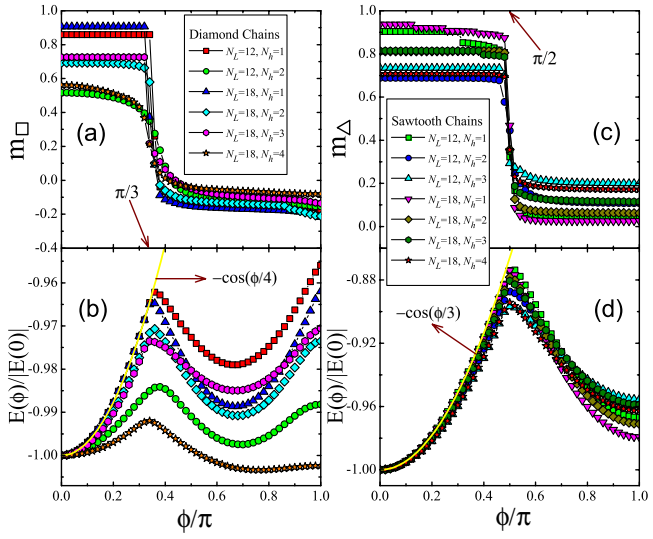

FIG. 2 (color online). (a),(b) Diamond chains. (c),(d) Sawtooth chains. m's and rescaled GS energies versus ϕ.

such a state (with $0 \leq \phi < \phi_c$) is referred to as a Nagaoka-type FM. When ϕ varies from ϕ_c to π, all m's show obvious intraplaquette AFM correlations ($m_\square < \frac{1}{4}$ for diamond chains, and $m_\triangle < \frac{1}{2}$ for sawtooth chains). Since $\phi = \pi$ corresponds to the HS's problem ($\mathcal{S}_{\text{loop}} = -1$) and m's change little as $\phi_c < \phi \leq \pi$, we also extend the notion of HS AFM and such a state (with $\phi_c < \phi \leq \pi$) is referred to as an HS-type AFM.

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

For the 8×2, 10×2 and 12×2 square ladders with respectively $N_h = 1$–3, $N_h = 2$–4 and $N_h = 1$–2, as seen from Figs. 3(a) and 3(b), the abrupt drops of $m_\square$'s and nonanalyticities in GS energies occur near different ϕ_c's, with ϕ_c versus hole density x varying rather smoothly.

For the 6×2 and 9×2 trestle ladders with respectively $N_h = 1$–3 and $N_h = 1$–4 [Figs. 3(c) and 3(d)], the abrupt drops of $m_\triangle$'s and nonanalyticities in GS energies also occur near different ϕ_c's, with still a smooth curve of ϕ_c versus x.

In these ladders, m's change very little and satisfy $m > \frac{1}{2}$ when ϕ varies from 0 to ϕ_c, the curves of rescaled GS energy are very close to that of $E^{\text{1h}}_{\text{FM}}(\phi)/|E^{\text{1h}}_{\text{FM}}(0)|$, and these states are of Nagaoka-type FMs; when ϕ varies from ϕ_c to π, all m's show obvious intraplaquette AFM correlations, and these states are of HS-type AFMs.

It is tempting to estimate ϕ_c in the limit of low hole density ($x \to 0$). Such a task can be partly fulfilled with the Brinkman-Rice (BR) approximation [17]. For a single hole in an infinite Néel AFM spin background, the BR approximation accounts the dominant contributions to the self energy of single-hole Green's function, i.e., the retraceable paths without any closed loop. Such an approximation leads to a hole band edge (i.e., the lowest single-hole kinetic energy) $E^{\text{BR}}_{\text{AF}} = -2\sqrt{z-1}$, where z is the coordination number.

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

Square and triangular lattices.—For the single-hole Nagaoka FM in an infinite square lattice with an SF, $E^{\text{1h}}_{\text{FM}}(\phi) = -4\cos(\phi/4)$; while for an infinite triangular lattice, $E^{\text{1h}}_{\text{FM}}(\phi) = -6\cos(\phi/3)$.

For the 4×4 and 6×4 square lattices with respectively $N_h = 1$–4 and $N_h = 1$–2 [Figs. 4(a) and 4(b)], or the 3×3 and 6×3 triangular lattices with respectively $N_h = 1$ and $N_h = 1$–3 [Figs. 4(c) and 4(d)], the abrupt drops of m's and nonanalyticities (or changes of concavities) in GS energies also occur near different ϕ_c's. In all these cases, the GSs are of Nagaoka-type FMs for $0 \leq \phi < \phi_c$, and are of HS-type AFMs for $\phi_c \ll \phi \leq \pi$. The curve of ϕ_c vs x of the square lattices [the inset in Fig. 4(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 [15].

A rough estimation of ϕ_c in the limit $x \to 0$ with the aid of the BR approximation is: $\phi^{\text{BR}}_c = 2\pi/3$ for an infinite

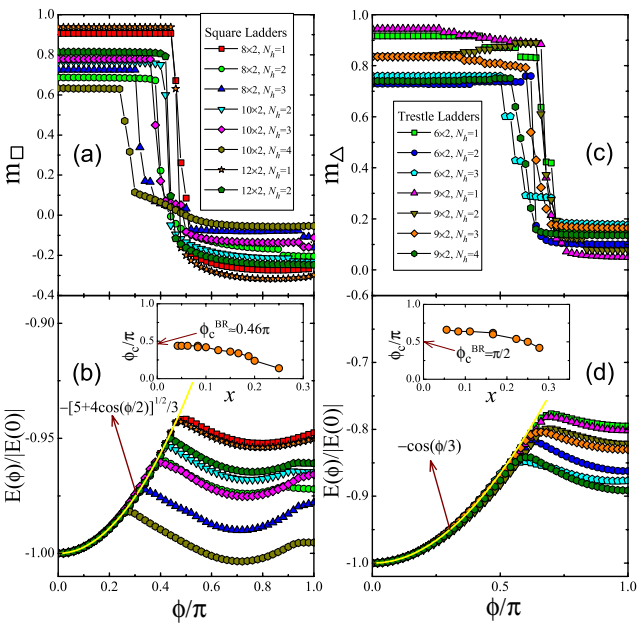

FIG. 3 (color online). (a),(b) Square ladders. (c),(d) Trestle ladders. m's and rescaled GS energies versus ϕ. The insets in (b) and (d) show ϕ_c vs hole density x.

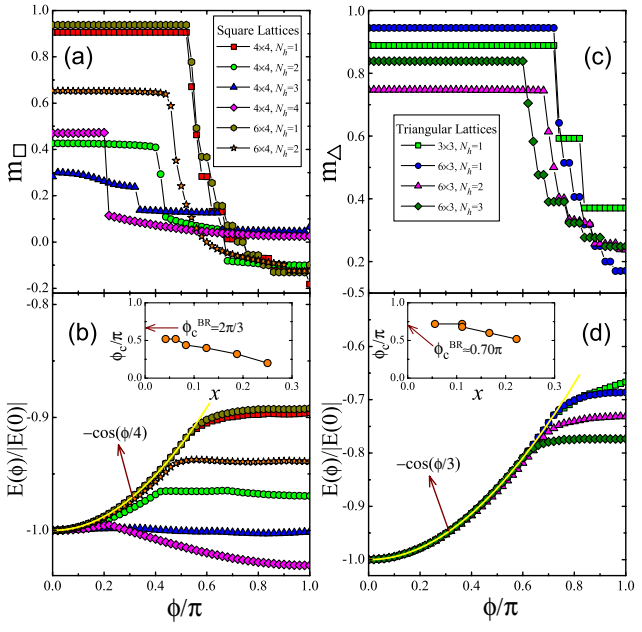

FIG. 4 (color online). (a),(b) Square lattices. (c),(d) Triangular lattices. m's and rescaled GS energies versus ϕ. The insets of (b) and (d) show ϕ_c vs hole density x.

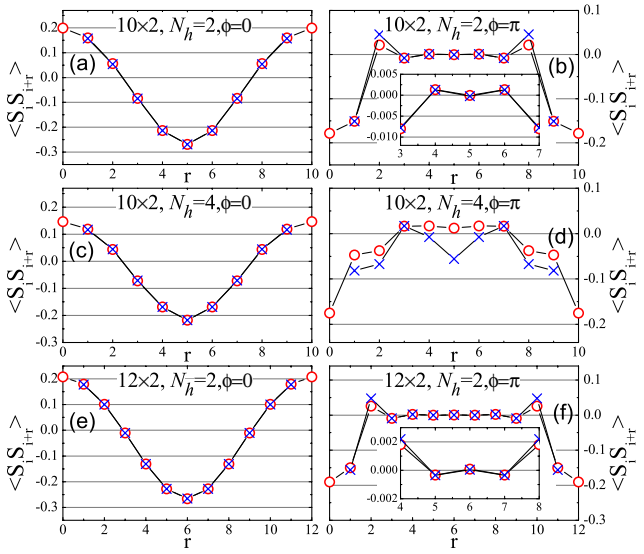

FIG. 5 (color online). Long-range intrachain (cross) and interchain (circle) spin correlations of square ladders at $\phi = 0$ and $\phi = \pi$. The insets in (b) and (f) enlarge the middle parts.

square lattice, and $\phi_c^{\mathrm{BR}} = 3\arccos(\sqrt{5}/3) \simeq 0.70\pi$ for an infinite triangular lattice.

Long-range spin correlations and ordering.—As seen from the above, m and $E(\phi)/|E(0)|$ describe well the transitions from a Nagaoka-type FM to an HS-type AFM. The ED data of the six kinds of lattices also tell us that for each case with odd N_h, the GS S_{tot} always takes the maximum value $N_e/2$ and $\langle S_i \cdot S_{i+r} \rangle$ is positive and almost a constant for any range r when $0 \leq \phi \ll \phi_c$, namely, the Naogaka-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 $N_h = 2$.

At $\phi = 0$ [Figs. 5(a), 5(c), and 5(e)], the GSs of the three cases are singlets ($S_{\mathrm{tot}} = 0$), however, there is an evidence of long-range FM in $\langle S_i \cdot S_{i+r} \rangle$ and each singlet GS actually consists of two FM domains with opposite magnetization as pointed out by Troyer *et al.* [14]. While at $\phi = \pi$ [Figs. 5(b), 5(d), and 5(f)], the GSs have decayed AFM correlations.

Summary and discussion.—An interplay between kinetic process and magnetic ordering has been demonstrated when strong correlation and electronic frustration are both present: (i) tuning ϕ from 0 to π makes the GS change abruptly from a Nagaoka-type FM to an HS-type AFM at a ϕ_c, with both states being metallic and of kinetic origin; (ii) this tunable kinetic magnetism is generic, and appears in various lattice structures with low hole densities ($x < 0.3$); (iii) at a ϕ_c, the intraplaquette spin correlation drops abruptly, and the GS energy exhibits nonanalyticity; (iv) the ϕ_c's of chains are insensitive to x, while the ϕ_c's of ladders or 2D lattices versus x exhibit a decreasing and almost smooth function; (v) a Nagaoka-type FM has long-range FM ordering, while an HS-type AFM has decayed AFM correlations.

Such results promise a novel physics in several future experimental systems. In an artificial lattice of quantum dots, interdot tunnelings $t \sim 0.01$ meV (and intradot Hubbard-like repulsion $U \sim 3$ meV) corresponding to lattice constants 300–500 nm [6] would enable us to observe this effect at a flux strength ~100 Gs. For a periodic net of carbon nanotubes connected by point tunneling contacts, segments of nanotubes between contacts would play the role of electron sites and contacts would determine the parameter t [7]. In optical lattices of ultracold atoms, appropriate phase factors can be introduced for hopping integrals by laser assisted tunneling, lattice tilting, or employing atoms with multiple internal states [8].

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