Violation of Luttinger's theorem in the simplest doped Mott insulator: Falicov-Kimball model in the strong-correlation limit

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Luttinger's theorem has long been taken as the key feature of Landau's Fermi liquid, which signals the presence of quasiparticles. Here, by the unbiased Monte Carlo method, violation of Luttinger's theorem is clearly revealed in the Falicov-Kimball (FK) model, indicating a robust correlation-driven non-Fermi-liquid characteristic under any electron density. Introducing hole carriers to the half-filled FK model leads to Mott insulator-metal transition, where the Mott quantum criticality manifests unconventional scaling behavior in transport properties. Further insight on the violation of Luttinger's theorem is examined by combining Hubbard-I approximation with a composite fermion picture, which emphasizes the importance of a mixed excitation of the itinerant electron and the composite fermion. Interestingly, comparing the FK model with a binary disorder system suggests that the two-peak band structure discovered by Monte Carlo and Hubbard-I approaches is underlying the violation of Luttinger's theorem.

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I. INTRODUCTION

Electron correlation has long been the key ingredient of modern condensed matter physics. In strongly correlated systems, such as the heavy fermion compound, cuprates, and iron-based superconductors, correlation introduces various unconventional metallic states [1-3]. The metallic state with linear-T resistivity is often called strange metal after its discovery in the normal state of high- T_c cuprates superconductors. Similar phenomena have also been found in heavy fermion compounds where the magnetic quantum critical point is approaching. These unconventional metallic states cannot be understood in the framework of Landau's Fermiliquid (FL) theory and have been empirically classified as non-Fermi liquids (NFLs) due to anomalous thermodynamic and transport properties [4]. Unfortunately, despite intensive decades of studies, our knowledge of generic NFLs (beyond artificial large-N limits or solvable models) is still very limited because the intrinsic strong-correlation effect is beyond the scope of Hartree-Fock mean-field and perturbation theory frameworks, thus intuitive understanding of these NFLs is largely unknown.

Fortunately, Luttinger's theorem provides a heuristic way to understand the essence of the NFLs, which writes as

$$\frac{N}{V} = 2 \int_{\text{Re}G(\mathbf{k},\omega=0)>0} \frac{d^d k}{(2\pi)^d},$$
 (1)

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for spinful systems [5]. The integral in momentum space is taken over the propagator at the Fermi energy where $\operatorname{Re}G(\mathbf{k}, \omega = 0)$ is positive (a more precise statement will appear later). Luttinger's theorem suggests the existence of quasiparticles and has long been taken as a key feature of FL. Recently, several numerical studies have confirmed that Luttinger's theorem is violated in the doped correlation-driven Mott insulators, e.g., in the Fermi-Hubbard model, t - V, model and t - J model [6–15]. However, the accuracy of these studies is affected by the dimension, size of the system, limited temperature region, and crude approximation. Especially for a doped Mott insulator lacking particle-hole symmetry, due to the notorious minus-sign problem, the most trustworthy determinant quantum Monte Carlo simulation of the Fermi-Hubbard model is limited to a small size and high temperature, whereas the analytical study can rarely predict the nature of a specific system. In our previous work, we have studied the violation of Luttinger's theorem in the anisotropic limit of the Kondo lattice, i.e., the Ising-Kondo lattice model [16]. Considering the specific feature of the Ising-Kondo lattice, the unbiased study of the violation of Luttinger's theorem is still insufficient and a more generic and transparent system that permits unbiased Monte Carlo simulation on a large size close to the thermodynamic limit is heavily desired.

We note that the Falicov-Kimball (FK) model is an ideal platform to study Luttinger's violation of the doped Mott insulator. The FK model is an alternative Hubbard model, which can be exactly solved within the framework of dynamical mean-field theory in infinite dimension [17]. Hitherto,

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most studies about the FK model are restricted to the weak coupling regime, where the long-range correlation and the natural tendency to phase separation conspire to rich patterns in the zero-temperature phase diagram [17,18]. These stripelike or inhomogeneous charge orderings can correspond to kinds of strongly correlated electron systems [19–21], such as the doped cuprates [22–32], layered cobalt oxides [33,34], and nickelates [35–39]. It used to be thought that the FK model in small interaction (use U as its strength) is more unconventional, while the large U situation can be simply mapped onto an effective Ising model, and thus its underlying physics has been rarely reported in literature [40]. In this paper, we instead focus on the strong coupling regime and reveal that the strong correlation leads to nontrivial quantum states beyond Landau's FL paradigm. At high temperatures, the FK system has no long-ranged charge order and thus could be clearly studied in terms of the violation of Luttinger's theorem. It was reported that the Anderson insulator can be induced by any finite correlation at the thermodynamic limit [41]. Here, we find that in the doped Anderson insulator with sufficient correlation $(U > U_c)$, the single band evolves into a robust two-band structure, with which Luttinger's theorem is violated. The disappearance of quasiparticles suggests the crossover from FL to NFL occurs in the Anderson insulator with increasing interaction. The evolution of band structure and the Luttinger integral (LI) can be exactly covered by a binary disordered system, with which we confirm the two-band structure is underlying the violation of Luttinger's theorem. Actually, not all the NFLs can violate Luttinger's theorem. When the Mott gap is absent, where the singleband structure in the NFL sustains under interaction, such as the Sachdev-Ye-Kitaev model, Luttinger's theorem is satisfied [42]. Combined with previous studies, for the specific NFLs arising from the doped Mott insulator, the NFL nature is attributed to the change of band structure, and this kind of NFLs can be confirmed by the violation of Luttinger's theorem.

The remainder of this paper is organized as follows: In Sec. II, the FK model is introduced and its phase diagram is briefly discussed. The strange metal state is demonstrated by the calculation of resistivity and specific heat. In Sec. III, we show that Luttinger's theorem is violated in the FK model in terms of direct numerical calculation. In Sec. IV, we provide some analytical results with the Hubbard-I approach and analyze it by the composite fermion. In Sec. V, with the assistance of Luttinger's theorem, the phase diagram in the U-T plane at half filling is elaborated. A binary disordered system is discussed. We compare the violation of Luttinger's theorem and the spectrum function between the disordered system and the FK model and end the paper with a summary.

II. MODEL AND METHOD

We consider the FK model [17] on a square lattice; the Hamiltonian is defined as

$$\hat{H} = -t \sum_{i,j} \hat{c}_i^{\dagger} \hat{c}_j + U \sum_i \hat{n}_i \hat{w}_i - \mu \sum_i \hat{n}_i, \qquad (2)$$

where $\hat{c}_{j}^{\dagger}(\hat{c}_{j})$ is the itinerant electron's creation (annihilation) operator at site *j*. $\hat{n}_{j} = \hat{c}_{j}^{\dagger}\hat{c}_{j}$ denotes the particle number of the itinerant electron, while \hat{w}_{j} denotes the particle number operator for the electron in the localized state. The *t* term denotes the hopping integral and only nearest-neighbor hopping is involved. *U* is the onsite Coulomb interaction between the itinerant electron and the localized electron. The hole doping into the half-filled system ($\mu = \frac{U}{2}$) is realized by tuning the chemical potential μ .

In Eq. (2) we neglect the chemical potential term $(-\mu_f \sum_i w_i)$ of the localized electrons. Note that $[\hat{w}_j, \hat{H}] = 0$, which means the number of localized electrons at each site is conservative ($w_i = 0$ or 1) for a specific chemical potential μ_f . Therefore, the localized electrons do not have any dynamic properties or the time-dependent Green's function, even if μ_f is included. The chemical potential of localized electrons will affect the properties of *c* electrons merely through changing the localized electron number. In this context we focus on the situation where the *f* electron is half filling to access a more nontrivial system (see Supplemental Material [43]).

Taking the eigenstates of the number operator of localized electron \hat{w}_j as bases, the Hamiltonian is automatically reduced to an effective free fermion model:

$$\hat{H}(w) = -t \sum_{i,j} \hat{c}_i^{\dagger} \hat{c}_j + U \sum_i n_i \hat{w}_i - \mu \sum_i n_i.$$
(3)

Here, w emphasizes its w dependence and $\hat{w}_i |w_i\rangle = w_i |w_i\rangle$, $w_i = 0, 1$. Now the many-body eigenstate of the original model can be constructed by the single-particle state of the effective Hamiltonian under a given configuration $\{w_i\}$, and thus the Monte Carlo simulation can be simply carried out. In this context, we consider the square lattice with periodic boundary conditions. The sampling using the truncation algorithm is used, with which we are able to carry on a simulation of the system as large as $N_s = 3600$ [44]. Since the thermodynamic and transport properties of the FK model have been studied in the literature, here we focus on the nature of the Fermi surface. Therefore, a 60×60 square lattice is mainly used in the calculation of LI, while the others are calculated with a 20×20 square lattice. Accordingly, the twodimensional Brillouin zone is sampled by a 60×60 k-point grid. The nearest-neighbor hopping integral is used as the unit (t = 1) to measure all energy scales. To attack the NFLs in the doped Mott insulator, we focus on the strong coupling regime (U = 10). In this paper, we dope the half-filled FK model and consider the hole-doping case by tuning the chemical potential μ . The translation from hole doping to electron doping is straightforward due to the particle-hole symmetry. Compared with the Hubbard model, due to the lack of spin degree of freedom, in the FK model the itinerant electron on each site contains only one possible state. The particle-hole symmetry also dictates that the particle density is $n_c = 0.5$ when $\mu = \frac{U}{2}$.

As indicated in the previous studies in Refs. [18,40,45], the low-temperature ordered states could be identified with structure factor $S_q^{\omega}(Q)$, correlation function g_n , and the renormalized correlation function G_n , which are respectively



FIG. 1. The phase diagram of the Falicov-Kimball (FK) model in the μ -T plane at U = 10. The nearest-neighbor hopping integral is used as the unit (t = 1) to measure all energy scales. The lowtemperature regime is divided into a charge density wave (CDW) state and phase separation (PS) state by a first-order transition. At high temperatures, there exists a Mott insulator state around the half-filling situation and three distinguishable non-Fermi-liquid (NFL) states. A quantum critical region is induced by doping-driven Mott insulator-metal transition. With increasing doped holes, the Mott insulator crosses over successively to the first non-Fermi-liquid (NFL-I) state, the strange metal (SM) state, and finally to the second non-Fermi-liquid (NFL-II) state.

defined as

$$g_{n} = \frac{1}{4N} \sum_{i=1}^{N} \sum_{\tau_{1}, \tau_{2}=\pm 1}^{w} w(\mathbf{r}_{i}) w(\mathbf{r}_{i} + \tau_{1}\hat{x} + \tau_{2}\hat{y}),$$

$$G_{n} = (-1)^{n} 4 (g_{n} - \rho_{i}^{2}),$$

$$S_{q}^{w}(\mathbf{Q}) = \frac{4}{N} \sum_{i,j} e^{i\mathbf{Q}(\mathbf{R}_{i} - \mathbf{R}_{j})} w_{i} w_{j},$$
(4)

where $\rho_i = \frac{N_f}{N_s}$ is the concentration of localized electrons. N_f and N_s are the numbers of lattice sites and localized electrons, respectively. The above-mentioned quantities reveal a charge density wave (CDW) state at a low temperature around the half-filling situation. Away from half filling, inhomogeneity is indicated by the charge distribution in real space, which has a finite density of state around the Fermi energy. As for high temperature, the phase is detected by the properties of transports, thermodynamics, and spectral function. Accordingly, we elaborate a phase diagram under strong coupling (U = 10) on the μ -T plane with rich quantum states. The result is summarized in Fig. 1, where three different kinds of NFLs are uncovered with distinguishable thermodynamics and transports. At high temperatures, around half filling correlation opens the gap and leads to the Mott insulator. Doping holes into the half-filled FK model drives the Mott insulatormetal transition accompanied by Mott quantum criticality. With decreasing particle density, the Mott insulator crosses over to the first non-Fermi-liquid (NFL-I) state, the strange metal state, and the second non-Fermi-liquid (NFL-II) state, subsequently. Actually, the resistivity displays unambiguous



FIG. 2. The SM behavior in the FK model. (a) Logarithm temperature dependence of the capacity heat coefficient C(T)/T. (b) The linear-*T* resistivity. (c) The quantum critical scaling behavior. In the quantum critical region, the resistivity satisfies the quantum critical scaling. The SM is the metal-like part and the NFL-I is referred to as the insulatorlike part.

bifurcating quantum scaling behavior:

$$\rho(T,\delta\mu) = \rho^*(T)f[T/T_0(\delta\mu)], \tag{5}$$

where $T_0(\delta\mu) = c |\delta\mu|^{zv}$, $\delta\mu = \mu - \mu^*(T)$, and $\mu^*(T)$ is the critical "zero field" trajectory corresponding to the "separatrix" line. $\rho^*(T)$ is calculated for $\mu = \mu^*(T)$ and f(x) denotes the unknown scaling function. The resistivity on the separatrix is almost independent of temperature. The NFL-I and the strange metal together comprise the quantum critical region [see Fig. 2(c)]. The insulatorlike branch and metallic branch

satisfy different scaling functions f but have the same critical exponent zv = 1.25. The NFL-I is near the Mott insulator and has insulatorlike features, where an upturn exists in the resistivity curves at low temperatures. The strange metal state with a lower electron density instead shows the metallic transport properties. In such a quantum critical region, the FK model transits from insulator to metal. As shown in Figs. 2(a) and 2(b), the strange metal state is confirmed with linear-T resistivity and logarithm heat capacity coefficient dependence. In metallic states, resistivity follows $\rho(T) = \rho_0 + AT^n$. Around the separatrix line of the quantum critical region, resistivity shows a quadratic dependence of temperature (n = 2) and turns to linear dependence (n = 1) when crossing over to strange metal. Further decreasing electron density, the scaling behavior is lost but linear-T resistivity sustains, which is referred to as the NFL-II state.

III. VIOLATION OF THE LUTTINGER THEOREM

Given the unconventional transports and thermodynamics, it is natural to explore the quasiparticle properties in the hightemperature regime of the FK model. To achieve this aim, we examine the validity of Luttinger's theorem [5,46–48], which states that if the Landau quasiparticle exists, the volume enclosed by the Fermi surface is consistent with its density of particles. Such theorem has been proved originally by Luttinger and Ward in terms of the Luttinger-Ward functional in the framework of perturbation theory [46,47], and later by Oshikawa's nonperturbative topological argument [48]. It now has been accepted as a key feature of FL. Mathematically, Luttinger's theorem defines the LI below,

$$\mathrm{LI} = \int_{\mathrm{Re}G(\mathbf{k},\omega=0)>0} \frac{d^d k}{(2\pi)^d},\tag{6}$$

and for general FL it must be equal to the density of particles (n_c) :

$$LI = n_c. (7)$$

Here, $G(\mathbf{k}, \omega)$ is the retarded single-electron Green's function and $\theta(x)$ is the standard unit-step function with $\theta(x > 0) = 1$ and $\theta(x < 0) = 0$.

Intuitively, if we use the momentum space single-particle state $|\mathbf{k}\rangle$, the particle density n_c can be obtained by integrating the Fermi-Dirac distribution function with the weight w(k) for each $|\mathbf{k}\rangle$:

$$n_c = \int w(k) \times f(k) \frac{d^d k}{(2\pi)^d}.$$
(8)

At zero temperature in a free system, every $|\mathbf{k}\rangle$ state has the same spectral weight w(k) = 1, and the Fermi distribution function f(k) is the unit-step function of energy $f(k) = \theta(-\epsilon_k)$. Thus, the particle density is equal to the proportion enclosed by the Fermi surface, which is the same as the LI, and naturally Luttinger's theorem is satisfied.

Note that the LI is the positive proportion of the real part of the retarded Green's function in the first Brillouin zone, mathematically equal to the proportion enclosed by the Fermi surface. Actually, for any system, the LI can be interpreted as the integral of the Fermi-Dirac distribution function with a



FIG. 3. Schematic picture of the violation of Luttinger's theorem. For a free system with specific filling, the volume of the Fermi surface can be constructed by Luttinger's theorem. The red circle denotes the Fermi surface of a free system. The white region is enclosed by the Fermi surface of the interacting system. Adiabatically turning on the interaction in the free system (left) with fixed particle density, the volume enclosed by the Fermi surface sustains as the free one until some critical coupling strength (middle). Under strong enough coupling (right), the interaction changes the volume enclosed by the Fermi surface from the free system. In fact, the violation of Luttinger's theorem suggests the NFL state has no quasiparticle which can be originated from the free system; we use the magnified grid in the Fermi surface to indicate changes in statistics.

constant weight w(k) = 1:

$$\mathrm{LI} = \int 1 \times f(k) \frac{d^d k}{(2\pi)^d},\tag{9}$$

which is the counting of the occupied $|\mathbf{k}\rangle$ state. According to Eqs. (8) and (9), the working of Luttinger's theorem suggests w(k) = 1, i.e., in momentum space every volume element $\frac{d^d k}{(2\pi)^d}$ can contain one electron. Thus the counting of the electron number is equal to the counting of the occupied $|\mathbf{k}\rangle$ state. The many-body state and the excitation can be described clearly by the wave vector \mathbf{k} , which is a characteristic of the quasiparticle picture.

As shown in Fig. 3, by adiabatically turning on the correlation, the free fermion system evolves into FL, with the $|\mathbf{k}\rangle$ state modified on the perturbative level. In the FL state, the correspondence between the original state and the final state is valid, although the dispersion relation is modified by interaction. The correspondence between the free system and the FL suggests the presence of quasiparticles, where the weight of each $|\mathbf{k}\rangle$ state is still invariant as w(k) = 1. Actually, although the volume of the new Fermi surface in FL is invariant, its shape should depend on the form of self-energy. With an isotropic interaction, the real part of self-energy in momentum space is also isotropic, leading to an invariant Fermi surface. Since the interaction in the FK model is isotropic, in its FL regime we expect a Fermi surface, the same as in a free system. However, with anisotropic interaction, the resultant self-energy is inhomogeneous in momentum space, and thus the Fermi surface can be deformed even within the FL (see the white region in the middle panel of Fig. 3). Even though the interaction may change the occupied $|\mathbf{k}\rangle$ state, if only w(k) = 1, the volume enclosed by the Fermi surface is invariant with fixed particle density. It suggests the key feature of FL is the invariant spectral weight.



FIG. 4. Spectral function at Fermi energy $A_{\mathbf{k}}(\omega = 0)$ (upper panel) and the real part of the Green's function at Fermi energy ReG($\mathbf{k}, \omega = 0$) (lower panel) in the FL (left panel, $U = 1, T = 0.2, n_c = 0.3$) and the SM state ($U = 10, T = 0.2, n_c = 0.3$, right panel). According to Luttinger's theorem, the Fermi surface of a free system with particle density $n_c = 0.3$ is denoted by the white circle. The location of the Fermi surface is in accordance with the zero values of the real part of the Green's function.

We emphasize that Luttinger's theorem is valuable for the study of exotic metallic states. Given a specific filling, Luttinger's theorem provides a method to reconstruct the Fermi surface of a free system with the same particle density. For a specific correlated system, we can confirm the presence of quasiparticles if its Fermi surface encloses the same volume as the free system. Figure 4 displays the imaginary and real part of the retarded Green's function of the FK model at $n_c = 0.3$ under different coupling strengths. The upper panel plots the c electron's spectral function $A_{\mathbf{k}}(\omega = 0)$ in the first Brillouin zone and the lower panel plots the real part of the Green's function $\operatorname{Re}G(\mathbf{k}, \omega = 0)$, both of which are plotted around the Fermi energy. Based on Luttinger's theorem, we utilize the particle density to plot the Fermi surface of a free system with the white line. Note that whether in the FL (left panel) or in the strange metal state (right panel) the location of the Fermi surface is always coincident with the zero values of the real part of the Green's function. This ensures that in the strange metal state the LI is equal to the proportion enclosed by the Fermi surface.

For a weak coupling situation (left panel, U = 1), the interacting Fermi surface coincides with the free system, suggesting an FL nature. As for the strong coupling situation (right panel, U = 10), the interacting Fermi surface becomes heavily deformed. The volume of the Fermi surface is greater than the free one, which involves more possible occupied $|\mathbf{k}\rangle$ states. As shown in the right panel of Fig. 3, when increasing the interaction, the correspondence between the original state in the free system and the final many-body state in NFL disappears at some critical coupling strength. This suggests that the average spectral weight decreases, $\overline{w(k)} < 1$, and on average a $|\mathbf{k}\rangle$ state can contain an electron number less than 1. For



FIG. 5. An overall illustration of the violation of Luttinger's theorem. The Luttinger integral (LI) vs density of electron n_c at T = 0.2. In FL (U = 1 and 2), the electron density and Fermi surface are in accordance with Luttinger's theorem. At stronger coupling (U = 4), the proportion of the first Brillouin zone enclosed by the Fermi surface deviates from the density of electrons for most doping regimes, thus confirming their NFL nature. Further increasing coupling strength leads to a stronger deviation (U = 10).

conventional fermions, the Pauli exclusion principle permits only one electron in a state, whereas in the NFL the strong interaction effectively increases the exclusion in statistics.

In Fig. 5, we demonstrate the overall LI with varying coupling strength and varying filling. As reference, two dotted black lines are plotted as $n_c = LI$ and $2 \times LI$. Here, $n_c = LI$ is the LI of a free system, around which Luttinger's theorem works well. At exactly half filling, Luttinger's theorem works well at any coupling strength, due to the existence of particle-hole symmetry. With increasing coupling strength, Luttinger's theorem sustains to U = 2. When U > 2 the violation emerges and the magnitude increases gradually with increasing interaction. The degree of deviation corresponds to the degree of deformation of the Fermi surface, compared with the free system. Note that for a specific coupling strength U, the particle density changes the degree of deviation, but the deviation/similarity of two Fermi surfaces is robust with doping. This robust violation corresponds to the rigid band structure of the FK model. It suggests a robust NFL-like nature for all paramagnetic phases in the phase diagram (see Fig. 1).

Actually for the lattice model with finite sites, the above momentum integral should be replaced by a discrete summation of the k-point grid. Frankly speaking, Eq. (8) is strictly valid only for zero temperature. Since interesting physics like NFLs and the strange metal behavior often exist at finite T, here we follow the recent quantum determinant Monte Carlo study on the doped Hubbard model in Ref. [7] and still use Eq. (8) to estimate the validity of Luttinger's theorem at finite temperature. As indicated in our previous work, at the high-temperature regime the thermal effect on the LI is small [16]. As shown in Fig. 5, at low-filling level LI displays a linear dependence of the particle density $LI = a \times n_c$ whereas $a \neq 1$ indicates the changes of statistics in NFLs. Here, the spectral weight is $w(k) = \frac{1}{a}$. The linear- n_c behavior sustains until some critical particle density, which is closely associated with the band structure. The critical n_c is correspondent to the coincidence of Fermi energy and the pseudogap. Not only the critical particle density ($n_c \approx 0.25$) but also the critical coupling strength ($U_c = 2$) all turn out to be closely related to the band structure. These properties will be further discussed in the binary disordered system in the final section.

IV. HUBBARD-I APPROXIMATION AND COMPOSITE FERMIONS ANALYSIS

In the last section, with unbiased Monte Carlo simulation, we study the violation of Luttinger's theorem in the FK lattice. In this section, we want to further study the microscopic mechanism of the violation of Luttinger's theorem analytically. In the high-temperature situation, one can follow the Hubbard-I approximation to give a rough solution for the FK model. At first, we use the equation of motion (EOM) formalism and define the retarded Green's function as [49]

$$G_{i,j,\sigma}(\omega) = \langle \langle \hat{c}_{i\sigma} | \hat{c}_{j\sigma}^{\dagger} \rangle \rangle.$$
(10)

By using the standard EOM relation,

$$\omega\langle\langle \hat{A}|\hat{B}\rangle\rangle_{\omega} = \langle [\hat{A},\hat{B}]_{+}\rangle + \langle\langle [\hat{A},\hat{H}]_{-}|\hat{B}\rangle\rangle_{\omega}.$$
 (11)

For the FK model, the Hamiltonian can be rewritten as

$$\hat{H} = -t \sum_{i,j} \hat{c}_i^{\dagger} \hat{c}_j + \frac{U}{2} \sum_i (2\hat{w}_i - 1)\hat{n}_i + \left(\frac{U}{2} - \mu\right) \sum_i \hat{n}_i.$$
(12)

In the half-filled situation, it follows that

$$\omega \langle \langle \hat{c}_i | \hat{c}_j^{\dagger} \rangle \rangle_{\omega} = \delta_{ij} - t \Delta_{im} \langle \langle \hat{c}_m | \hat{c}_j^{\dagger} \rangle \rangle_{\omega} + \frac{U}{2} \langle \langle (2\hat{w}_i - 1)\hat{c}_i | \hat{c}_j^{\dagger} \rangle \rangle_{\omega}.$$
(13)

Here, Δ_{im} denotes that *m* is the nearest-neighbor site of *i*. For $\langle \langle (2\hat{w}_i - 1)\hat{c}_i | \hat{c}_i^{\dagger} \rangle \rangle_{\omega}$, we have

$$\omega \langle \langle (2\hat{w}_i - 1)\hat{c}_i | \hat{c}_j^{\dagger} \rangle \rangle_{\omega} = \langle (2\hat{w}_i - 1) \rangle \delta_{ij} - t \Delta_{il} \langle \langle (2\hat{w}_i - 1)\hat{c}_l | \hat{c}_j^{\dagger} \rangle \rangle_{\omega} + \frac{U}{2} \langle \langle \hat{c}_i | \hat{c}_j^{\dagger} \rangle \rangle_{\omega}.$$
(14)

If no further EOM is involved, to close the EOM we have to decouple $\langle \langle (2\hat{w}_i - 1)\hat{c}_l | \hat{c}_i^{\dagger} \rangle \rangle_{\omega}$ as

$$\langle \langle (2\hat{w}_i - 1)\hat{c}_l | \hat{c}_j^{\dagger} \rangle \rangle_{\omega} \simeq \langle 2\hat{w}_i - 1 \rangle \langle \langle \hat{c}_l | \hat{c}_j^{\dagger} \rangle \rangle_{\omega}.$$
(15)

In the paramagnetic strong coupling regime, there is no finite CDW order, thus $\langle (2\hat{w}_i - 1) \rangle = 0$. Meanwhile, the contribution from $\langle \langle (2\hat{w}_i - 1)\hat{c}_i | \hat{c}_j^{\dagger} \rangle \rangle_{\omega}$ vanishes due to the decoupling and the above equation has a complete solution:

$$\left(\omega - \frac{U^2}{4\omega}\right) \langle \langle \hat{c}_i | \hat{c}_j^{\dagger} \rangle \rangle_{\omega} = \delta_{ij} - t \,\Delta_{im} \langle \langle \hat{c}_m | \hat{c}_j^{\dagger} \rangle \rangle_{\omega}, \qquad (16)$$

which can be written as

$$\left(\omega - \frac{U^2}{4\omega}\right)G_{i,j}(\omega) = \delta_{ij} - t\,\Delta_{im}G_{m,j}(\omega). \tag{17}$$

Now, performing the Fourier transformation

$$G_{i,j}(\omega) = \frac{1}{N_s} \sum_{k} e^{ik(R_i - R_j)} G(k, \omega), \qquad (18)$$



FIG. 6. LI vs density of electron n_c at T = 0.2. It displays the violation of Luttinger's theorem by Monte Carlo simulation (blue, U = 10) and the Hubbard-I approximation method (orange, U = 10), respectively. The LI of the free fermion system (yellow) is plotted as a reference.

we have

$$\sum_{k} \left(\omega - \frac{J^2}{16\omega} \right) G(k, \omega) e^{ik(R_i - R_j)}$$
$$= \sum_{k} e^{ik(R_i - R_j)} - t \Delta_{im} G(k, \omega) e^{ik(R_m - R_j + R_i - R_i)}.$$
(19)

Here, $-t\Delta_{im}e^{ik(R_m-R_i)} = -t\sum_{\delta}e^{-ik\delta} = \varepsilon_k$ and we have $\sum_k [(\omega - \frac{U^2}{4\omega})G(k,\omega) - 1]e^{ik(R_i-R_j)} = 0$, which gives the single-particle Green's function as

$$G(k,\omega) = \frac{1}{\omega - \frac{U^2}{4\omega} - \varepsilon_k} = \frac{\alpha_k^2}{\omega - \hat{E}_k^+} + \frac{1 - \alpha_k^2}{\omega - \hat{E}_k^-}.$$
 (20)

Here, the coherent factor $\alpha_k^2 = \frac{1}{2}(1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + U^2}})$ and

$$\hat{E}_k^{\pm} = \frac{1}{2} \left[\varepsilon_k \pm \sqrt{\varepsilon_k^2 + U^2} \right]. \tag{21}$$

With the above single-particle Green's function, we plot the LI at U = 10 by the Hubbard-I approximation (orange line with circle marker) as a function of particle density and compare it with the Monte Carlo result (blue line with circle marker) in Fig. 6. As a reference, the LI of the free fermion system is plotted in a yellow line with a circle marker.

It turns out that the Hubbard-I approximation provides an accurate evaluation for the Fermi surface at a strong coupling regime. This agreement between results of the Hubbard-I approximation and the Monte Carlo simulation is reasonable, since the system is under a strong-correlation limit, where the energy scale of the interaction (U/t = 10) is much larger than the temperature (T/t = 0.2). Compared with the situation in the Hubbard model, in the FK model the Hubbard-I approximation works better, which can almost recover the violation of Luttinger's theorem. This advantage in the FK model is attributed to the commutation between the interaction and hopping terms

$$[2\hat{w}_i - 1, \hat{c}_i \hat{c}_i^{\dagger}] = 0, \qquad (22)$$

where the EOM truncates naturally at the second order only if we assume Eq. (15) works.

As mentioned above, the violation of Luttinger's theorem suggests the correspondence between FL and NFL is lost. We cannot access an approximated formalism of the quasiparticle by renormalizing parameters, such as the effective mass. This reminds us that an unconventional type of quasiparticle (not Landau quasiparticle) excitation should be expected, only if it exists. To access an intuitive understanding of the violation of Luttinger's theorem in terms of an approximated quasiparticle, we provide a composite fermion approach with a similar result compared with the Hubbard-I approximation. We note that the interaction term in Eq. (2) can be interpreted as the hybridization between the itinerant electrons and some composite fermions $f_j^{\dagger} = (2\hat{w}_j - 1)c_j^{\dagger}$, which satisfies the commutation relation of fermions

$$\{f_i^{\dagger}, f_j\} = (2\hat{w}_i - 1)(2\hat{w}_j - 1)\{c_i^{\dagger}, c_j\} = \delta_{ij}.$$
 (23)

However, the commutation relation between the composite fermion and the itinerant electron is nontrivial:

$$\{c_i^{\dagger}, f_j\} = (2\hat{w}_j - 1)\{c_i^{\dagger}, c_j\} = (2\hat{w}_j - 1)\delta_{ij}.$$
 (24)

Now the FK Hamiltonian can be written as

$$\hat{H} = -t \sum_{i,j} \hat{c}_{i}^{\dagger} \hat{c}_{j} + \frac{U}{4} \sum_{i} (\hat{f}_{i}^{\dagger} \hat{c}_{i} + \hat{c}_{i}^{\dagger} \hat{f}_{i}) + \left(\frac{U}{2} - \mu\right) \sum_{i} \hat{n}_{i}.$$
(25)

We assume $\{c_i^{\dagger}, f_j\}$ can be replaced by its average value. At the high-temperature paramagnetic regime $\langle (2\hat{n}_j - 1) \rangle = 0$ and thus the composite fermion and itinerant electron restore a standard commutation relation $\{c_i^{\dagger}, f_j\} = 0$. It suggests at high temperatures we can treat the composite fermion as a conventional fermion. By Fourier transformation, the Hamiltonian can be written as

$$\hat{H} = \sum_{k} (\hat{c}_{k}^{\dagger} \hat{f}_{k}^{\dagger}) \begin{pmatrix} \epsilon_{k} + \frac{U}{2} - \mu & \frac{U}{4} \\ \frac{U}{4} & 0 \end{pmatrix} \begin{pmatrix} \hat{c}_{k} \\ \hat{f}_{k} \end{pmatrix}.$$
(26)

The dispersion is given by diagonalizing the Hamiltonian:

$$\hat{E}_k^{\pm} = \frac{1}{2} \bigg[\varepsilon_k \pm \sqrt{\varepsilon_k^2 + \frac{U^2}{4}} \bigg].$$
(27)

This dispersion is similar to the Hubbard-I results, with a gap $\Delta E = \frac{U}{2}$ smaller than $\Delta E_{\text{Hubbard-I}} = U$. This composite fermion phenomenologically suggests that the elementary excitation of the FK model consists of the contribution of both the itinerant electron and the composite fermion. Therefore, it is hard to describe the many-body state in terms of a single (Landau) quasiparticle picture. As particle number increases by 1, the correspondent many-body state of the momentum space occupied a volume larger than $\frac{d^dk}{(2\pi)^d}$. However, the drawback of the composite fermions picture is also obvious. The composite fermions picture can merely provides an intuitive qualitative analysis. One can apply it also in one dimension, but we know that there the FL state is broken through charge-spin separation, not formation of composite fermions.

V. DISCUSSION AND CONCLUSION

We note the robust violation/working of Luttinger's theorem for a specific coupling strength in the doped FK model,



FIG. 7. The phase diagram of the FK model in the U-T plane at a half-filling situation. The low-temperature regime is a CDW state under any finite coupling. At high temperatures, three different states are uncovered. Under weak coupling the system sustains as an FL until U = 2. At moderate coupling, the Anderson insulator (AI) emerges with a crossover. Further increasing correlation leads to the MI with a fully opened energy gap.

which is invariant under different doping. Therefore, Luttinger's theorem can not only help tell NFLs from FLs in the doped system, but also help distinguish different states under different coupling strengths at half filling, although the working of Luttinger's theorem is protected there by the particle-hole symmetry. According to the order parameter in Eq. (4), the density of state, the inverse participation ratio, and the critical coupling strength where Luttinger's theorem fails with doping, the half-filling phase diagram of the FK model in the U-T plane can be elaborated as in Fig. 7. At low temperatures, the CDW state exists under any finite interaction U. At high temperatures, under strong coupling (U > 6), the FK model is a Mott insulator with a fully opened energy gap. Under weak coupling (U < 2), the FL nature sustains. Under a moderate coupling (2 < U < 6), there exists a finite density of state around Fermi energy while the two-band structure emerges. The localization revealed by the inverse participation ratio suggests an Anderson insulator.

Note that the phase diagram is different from the previous one in Ref. [41]. In Ref. [41], the whole metallic regime is indicated as the localization state, where the Anderson insulator state can be extrapolated to any finite small coupling at the thermodynamic limit. In this paper, according to the critical coupling strength where Luttinger's theorem is violated in the doped FK lattice, we find that the Anderson insulator state can be further divided into an FL state at weak coupling and an NFL state at strong coupling. Moreover, the FL state is not simply the effect of finite size, which can sustain to $U \approx 2$ at the thermodynamic limit.

Since the Anderson localization in the FK model has long been attributed to the disorder effect [50], it is valuable to check the pure effect of disorder on the working of Luttinger's theorem. We wonder whether increasing the strength of disorder will lead to the disappearance of quasiparticles. Since the doped FK model possesses a robust rigid two-band structure at strong coupling, some connection may exist between the robust violation of Luttinger's theorem and the robust twoband structure, which also corresponds to the singularity of



FIG. 8. (a)–(c) Density of state under different coupling/disorder strength at $n_c = 0.3$ at high temperature T = 0.2. The density of state of the FK model is denoted by the blue line, and the binary disordered system is denoted by the red line. (d) In the FK model, the energy gap is opened under small interaction U = 1 at low temperature T = 0.01. This opened gap can easily be erased by either thermal fluctuation or doping holes.

the Green's function at the high-energy regime [51]. However, we wonder whether the origin of band splitting is also important. To this end, it is necessary to study a disordered system, which could induce a two-band structure in the absence of interaction. Thus, in this section, we construct a Hamiltonian with interaction replaced by the discrete binary disorder to study Luttinger's theorem in a two-band system, which is written as

$$\hat{H} = -t \sum_{i,j} \hat{c}_i^{\dagger} \hat{c}_j - \sum_i (\mu_i - \mu_0) \hat{n}_i.$$
(28)

Different from the FK model, where μ is fixed during a Monte Carlo simulation, in this disordered system chemical potential is composed of two parts and the binary disorder is introduced by μ_i . For each site *i*, μ_i is randomly taken as $\mu_i = \pm U_{\text{disorder}}$. μ_0 instead is a fixed number in Monte Carlo simulation and it is used to tune the particle density.

We show the density of state at $n_c = 0.3$ for this disordered system (red line) with different disorder strengths in Figs. 8(a)-8(c) and compare it with the FK model (blue line). It turns out that when $|\mu_i| = U_{\text{FK}}$, $\mu_0 = \mu_{\text{FK}} - \frac{U_{\text{FK}}}{2}$, the spectral function of the FK model agrees with the disordered system perfectly with varying coupling/disorder strength U. Even the locations of the pseudogaps are in accordance with each other. At small coupling/disorder strength (U = 1), only one quasiparticle peak exists and it is the same with the free electron situation. Under a moderate coupling strength (2 < U < 6), the two-peak structure emerges while the gap is



FIG. 9. LI vs density of electron n_c at T = 0.2. It displays the violation of Luttinger's theorem in the binary-disordered system. Within a weak disorder ($U_{\text{disorder}} = 1$ and 2), the system behaves as a general FL, where the electron density is in accordance with Luttinger's theorem. Within stronger disorder ($U_{\text{disorder}} = 4$), the doped Anderson insulator shows the NFL nature, where the proportion enclosed by the Fermi surface deviates from the density of electrons for the majority doping regime. Further increasing disorder strength leads to a stronger deviation ($U_{\text{disorder}} = 10$).

still not fully opened. The finite density of state around the Fermi energy and the two-peak structure leads to the localization of the FK/disordered system. This region is referred to as the Anderson insulator. Increasing coupling/disorder strength makes the gap fully opened, and the scale can be tuned by the magnitude of U.

As shown in Fig. 9, we further demonstrate the LI in the disordered system, as a function of disorder strength and particle density. We study the working/violation of Luttinger's theorem and the evolution of the spectral function at different parameters, to confirm the role that the band structure plays in the violation of Luttinger's theorem. As shown in Fig. 8(a), when the one-band structure sustains (U = 1), Luttinger's theorem works well where the Fermi surface enclosing a volume consistent with the particle density n_c (see Fig. 9). Increasing the disorder (U = 4) opens an energy gap $\Delta E \sim U$ in the middle of the spectrum and introduces the deviation of LI, suggesting a deformed Fermi surface with a larger enclosed volume. Note that at U = 4 the FK model is in the Anderson insulator state, where the gap is not fully opened. It indicates that the violation of Luttinger's theorem is directly caused by the two-peak structure, i.e., by the singularities of the self-energy at both high and low frequencies, rather than by the fully opened Mott gap. Further increasing the disorder (U = 10) leads to greater deviation and finally accesses the Mott insulator at half filling.

The LI in Fig. 9 is similar to the FK one shown in Fig. 5. In both the FK model and the disordered system, the working of Luttinger's theorem depends on the band structure. We want to emphasize that if the Anderson localization is introduced by the Gaussian-type disorder instead of this discrete disorder, Luttinger's theorem will not be violated due to the absence of a two-band structure. Therefore, we conclude that the NFL nature is not caused by localization.

As a function of particle density, the behavior of LI is associated closely with the characters of the spectrum

function, e.g., another singularity around the pseudogap. In both U = 10 and 4 situations, the LI displays a linear dependence of particle density when $n_c < 0.25$, where $n_c = 0.25$ is correspondent to the filling around the pseudogap.

The previous study based on cluster dynamical mean field theory suggests that the FK model is never a strict Landau FL even at a weak coupling situation $(U/t \approx 0.5)$ [52]. However, our paper indicates that Luttinger's theorem is working perfectly at U/t = 1 as shown in Fig. 4, which instead is a clear signal for the presence of the quasiparticle. The disagreement originates from the fact that the NFLs we discussed here are embedded in high-temperature paramagnetic regimes, where the effect of thermal fluctuation plays an important role. Actually, as shown in Fig. 8(d), the CDW ground state of the FK model is robust for any finite U, in which the interaction splits the energy band and leads to a fully opened gap. However, different from the real NFLs, this two-band structure is not robust and can be simply destroyed by either thermal fluctuation or doping holes. Therefore, only conventional FL is revealed under weak coupling. Only if the coupling strength is larger than the critical value U_c ($U_c = 2$) can the energy gap sustain under thermal fluctuation and doping.

In this paper, with unbiased Monte Carlo simulation, we reveal an unambiguous violation of Luttinger's theorem in the doped FK model. Under strong coupling, doping holes in the half-filling FK lattice leads to a Mott insulator-metal transition. Intriguingly, the NFL nature is robust under strong coupling at any finite doping. As shown in Fig. 1, at high-temperature regimes three different NFLs are revealed. Empirically, we used to distinguish the NFL features by unconventional transport and thermodynamic properties, such as the linear-T resistivity and logarithm dependence of the heat capacity coefficient in the strange metal state. Al-

though demonstrating various thermodynamical and transport behaviors, their NFL-like nature does originate from a common ground in the spectrum. Here, with Luttinger's theorem, we demonstrate the deformation of the Fermi surface in the NFLs is associated with the transfer of spectral weight. After reliable numerical simulation, we try to analytically access the violation of Luttinger's theorem. With the Hubbard-I approximation approach where we have solved the EOM to the second order, the violation of Luttinger's theorem is reproduced quantitatively. To provide a more intuitive picture, we construct the composite fermion. It turns out that the excitation in the FK model is mixed of the itinerant electron and the composite fermion, which cannot be simply described by elementary excitation formalism of a specific particle. Considering the lack of quasiparticles, the breakdown of the FL paradigm is predictable. Finally, a binary disordered model is constructed to discuss the connection between the violation of Luttinger's theorem and the feature of the spectrum. This disordered system can cover the density of states in the FK model perfectly. In such a different model which emphasizes the disorder effect rather than interaction, the two-band structure can also deform the Fermi surface directly. In conclusion, the violation of Luttinger's theorem in the doped Mott insulator is directly connected to the two-band structure, where the change of statistics can be taken as the key feature of NFLs underlying unconventional phenomena.

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