Doped Orthogonal Metals Become Fermi Arcs

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Orthogonal metal and semi-metal are recently discovered unconventional metallic states originated from strongly correlated lattice models. They are orthogonal to the established paradigm of Landau’s Fermi-liquid (FL) in the sense that they acquire no Fermi surface (FS) but still conduct electronically and respond magnetically, and are therefore expected to hold the key of understanding experimental observations of non-Fermi-liquids – ranging from high-temperature superconductors to twisted graphene heterostructures. Here, we go a step further by doping the orthogonal semi-metal state in the lattice model, and unveil via unbiased quantum Monte Carlo simulation that the doped orthogonal semi-metal becomes Fermi arcs that go completely beyond the Luttinger sum-rule with broken FS but no symmetry breaking. The Fermi arcs coexist with a background of deconfined $Z_2$ gauge field, and we find the confinement transition as well as the hopping of the gauge-neutral composite fermion will bring the ‘large’ FS back upon approaching a FL phase. The entire phase diagram that contains Fermi arc metal, deconfined FL and confined FL are mapped out in unbiased manner.

INTRODUCTION

As the cornerstone of condensed matter physics, Landau’s Fermi liquid (FL) theory states that at zero temperature, a Fermi liquid has a closed Fermi surface (FS) marked by the momenta of gapless quasiparticle excitations, similar to its noninteracting counterpart. When the electron number is held fixed, the volume inside the FS is invariant upon interaction, this is the so-called Luttinger’s theorem (LT) [1], and the perturbative argument has been modernized from a topological perspective [2–4]. Under these guidelines, the volume inside the FS is conserved even in an interacting FL, and the reduction of FS must come from the breaking of symmetries which enlarges the elementary unit cell of the problem at hand.

Given the stringent requirement of LT, the ample experimental observations of correlated electron systems that obviously violate the relation between the volume of quasiparticle FS and the electron filling therefore post a serious challenge and show how little we actually know about the interacting metallic states. These systems are in general dubbed non-Fermi liquid (nFL) – ranging from the Cu-, Fe-, Cr- and Mn-based superconductors [5–10], heavy fermion compounds [11–16], to the recently discovered twisted graphene heterostructures [17–20]. In particular, the experimental observation of Fermi arcs [21–26], where the FS in underdoped cuprates does not form a continuous contour in momentum space but breakup into disconnected arcs, and shrink with decreasing temperature and collapse to the point nodes below $T_c$, offers the clearest violation of the Luttinger’s theorem and still await a well-accepted explanation.

Many theoretical proposals have been put forwarded over the decades to address Fermi arcs in specific and nFLs in general, such as the fluctuations of the d-wave pairing [27], competing order with superconductivity [28], finite-temperature life-time effects [29], the fractionalized FL* phase [3, 30–33] and SYK type of nFL [34–36], where the latter two are shown to exist by recent quantum Monte Carlo (QMC) simulations [37, 38]. And the violation of the Luttinger counting has been seen in 16-site DCA simulation of doped Hubbard model [39]. However, it is fair to say that until the present days, there exist no lattice realization of a strongly correlated model at generic fillings which can be unambiguously shown to give rise Fermi arcs. In particular, the FL* phase still has a closed Fermi surface, enclosing an area that is different from the prediction of the LT by half of the Brillouin Zone (BZ), with the other half taken by fractionalized excitations to conserve the total momentum [3, 30], whereas a state with Fermi arcs has discontinuous Fermi surfaces and a Luttinger volume cannot even be defined.

This is the knowledge gap we would like to fill in. Here we show, that a finite-temperature Fermi arc state at generic filling can be constructed in a lattice model of correlated electrons and observed with unbiased large-scale QMC simulations. The state of Fermi arc can indeed happen without any symmetry-breaking, and therefore appears to violate the Luttinger theorem, and consistent with the experimental signatures of Fermi surface reconstruction in cuprate materials in the underdoped regime. Just like the Fermi arc state in cuprate materials, the
FIG. 1. Spectral function $A(k, \omega = 0)$ and spin susceptibility $\chi(q, \omega = 0)$. The parameters are $L = 20, T = 0.05, \mu = 1.2$ and $g = 0.5$ with $t = 0.2$ (filling $n = 1.13$) in (a), (b) and $t = 1.0$ (filling $n = 1.11$) in (d), (e). The blue, yellow and green squares are the representative momenta at nodal ($\frac{3\pi}{5}, \frac{3\pi}{5}$) and antinodal ($\frac{3\pi}{5}, 0$ and $\frac{4\pi}{5}, 0$) directions. The quasiparticle fractions at these points are analyzed in Fig. 4. The Fermi arcs are seen in (a) and (d), (b) shows the $c$-fermion spin susceptibility $\chi(q, \omega = 0)$ inside the Fermi arc phase, (c) shows the spin susceptibility for doped free $\pi$-flux Dirac cones to the same filling as in (b). They acquire the same magnetic response meaning that the Fermi arc phase has a hidden FS of $f$-fermions with the same shape of doped Dirac cone. (e) shows the $c$-fermion spin susceptibility for the large FS case and (f) shows that of free Hamiltonian $H = -\sum_{i,j}(t_{ij}f_{i,\alpha}^\dagger f_{j,\alpha} + h.c.) - \mu \sum_i f_{i,\alpha}^\dagger f_{i,\alpha}$ with NN and NNN hoppings and tuned to the similar shape. The fermionic spin susceptibility in (e) stems from contributions of both $f$-fermion and $c$-fermion, and it is slightly different from the $\chi(q, \omega = 0)$ in (f) which only comes from the free large FS with the shape of (d), but they share the same shape.

Fermi arcs discovered here are finite-temperature phenomenon. The true ground-state of our model is an orthogonal metal with a hidden Fermi surface. At zero temperature, such an orthogonal-metal phase actually satisfies an extended variant of the LT, where a volume equal to one half of the BZ disperses because of an odd Ising gauge field, while the rest of the Luttinger volume goes into pockets of hidden Fermi surfaces, formed by fractionalized quasiparticles carrying gauge charge.

The lattice model we constructed, is comprised of fermion matter field, Ising matter field and they are minimally coupled to a $Z_2$ gauge field. We found that by doping the fermion matter field away from half-filling, Fermi arcs could result and coexist with a background of deconfined $Z_2$ gauge field. The Fermi arc phase with broken FS can transition into 'large' FS that respects the LT, either via the enhancement of the hopping of the gauge-neutral composite fermions or via the confinement of the $Z_2$ gauge field. The QMC simulation reveal that the transitions from Fermi arc to 'large' FS look continuous, and in the entire phase diagram that contains Fermi arc metal, deconfined FL and confined FL there exist no symmetry breaking of any kind. These findings offer the first realization of the Fermi arc phase from a lattice model at generic filling in unbiased manner.

**MODEL AND FERMI ARCS**

Our model, inspired by the proposal and recent realizations of orthogonal fermion construction [40–43], has the following Hamiltonian on a 2D square lattice,
FIG. 2. Lattice model, phase diagram and schematics for Fermi arc and FL states. (a) The lattice model in Eq. (1), on a square lattice, there are composite fermions $c_{i,\alpha} = f_{i,\alpha} S^{z}_{i}$ on each site $i$, comprised of orthogonal fermion field $f_{i,\alpha}$ and Ising matter field $S^{z}_{i}$. The $Z_2$ gauge field $\sigma_{b}^{z}$ lives on the bond $b$. The blue ellipse is the composite fermion, the combination of orthogonal fermion and spin field. (b) $t - g$ phase diagram of the model. At $g < g_c$ and $t < t_c$, the Fermi arc state is obtained by doping the OSM (orthogonal semi-metal). $g > g_c$ and $t > t_c$, the deconfined FL phase with $Z_2$ topological order coexists with large FS. At $g > g_c$, the $\pi$-flux state of the $Z_2$ gauge field is confined and the fermion then forms a conventional confined FL with large FS. (c) The red pockets are the hidden $f$-fermion FS inside the fermi arc phase ($g < g_c, t < t_c$), undetectable through single-particle spectra, but can be inferred from the spin susceptibility data Fig. 1 (b). The blue arcs are the Fermi arc in this phase that can be detected from experiments such as ARPES. (d) The blue circle is the $c$-fermion large FS inside both the deconfined and confined FL phases.

$$H = H_f + H_z + H_g + H_c,$$

$$H_f = - \sum_{\langle i,j \rangle} \left( f_{i,\alpha}^\dagger \sigma_{\delta,\langle i,j \rangle}^{\pi} f_{j,\alpha} + h.c. \right) - \mu \sum_i f_{i,\alpha}^\dagger f_{i,\alpha},$$

$$H_z = J \sum_{\langle i,j \rangle} S^z_i \sigma_{\delta,\langle i,j \rangle}^\pi S^z_j - h \sum_i S^x_i,$$

$$H_g = K \prod_{\mathcal{b}} \prod_{\mathcal{c}} \sigma^z_{\mathcal{b}} - g \sum_i \sigma^z_{\mathcal{b}},$$

$$H_c = - t \sum_{\langle i,j \rangle} f_{i,\alpha}^\dagger S^z_i f_{j,\alpha} S^z_j + h.c..$$

(1)

The model is depicted in Fig. 2 (a) with the parameters simplified in the following manner: $H_f$ is the orthogonal fermion part, with nearest neighbor (NN) hopping amplitude set at unity, the chemical potential $\mu$ controls the filling of the $f$ fermions and $\alpha = \uparrow, \downarrow$ is the spin index; $H_z$ is the Ising matter field part, with NN antiferromagnetic interaction $J = 0.1$ and the transverse field $h = 0.25$ to add quantum fluctuations; $H_g$ is the $Z_2$ gauge field part, with $K = 1$ such that $\pi$-flux per plaquette $\mathcal{b}$ is favored, and $g$ triggers the deconfinement-confinement transition of the gauge field. The last term, $H_c$, defines the NN hopping of the physical – gauge neutral – composite fermion $c_{i,\alpha}^\dagger (c_{i,\alpha}) = f_{i,\alpha}^\dagger S^z_i (f_{i,\alpha} S^z_i)$, denoted as the blue ellipse in Fig. 2, and we tune $t$ to enhance the $c$-fermion hopping such that the Fermi arc to 'large' FS transition can be realized. The quantum Monte Carlo implementation of this model, and with the $H_c$ term that requires block update scheme, is present in detail in the Supplemental Material [44].

As shown in previous works [42, 43], at half-filling of the $f$-electrons ($\mu = 0$), the zero-flux of the $Z_2$ gauge field can give rise to an orthogonal metal state in which the FS of the $c$-fermions vanishes with their quasiparticle fraction reduced to zero. And the $\pi$-flux of the $Z_2$ gauge field produces an orthogonal semi-metal state in which the FS of the $c$-fermions reduce to four Dirac points located at the nodal point $(\pm \pi, \pm \pi)$ of the BZ. Here we start from the orthogonal semi-metal state but tune the chemical potential $\mu$ away from half-filling.

The most striking results are show in Fig. 1. These are simulation results for $L = 20$, $T = 0.05 (\beta = 20), g = 0.5$, where we first contrast the Fermi arcs inside the doped orthogonal semi-metal phase in Fig. 1 (a) (with $t = 0.2$) with the large FS inside the deconfined FL phase in Fig. 1 (d) (with $t = 1$). The $c$-fermion spectral function can be approximated via its Green’s function as $A(k, \omega = 0) \propto \beta G(k, \beta / 2)$. The chemical potential in both cases are at $\mu = 1.2$ and their corresponding fillings are $n = 1.13$ and $n = 1.11$. At such filling, the large FS in Fig. 1 (d) respects the LT and the Fermi arc in Fig. 1 (a) certainly violates it. Later on we will show that the Fermi arc state indeed acquires broken FS with vanishing spectral weight at the BZ boundaries.

Fig. 1 (b) and (c) are the magnetic response of the Fermi arc metal and FL metal in Fig. 1 (a) and (d). We measure the magnetic susceptibility of the $c$ fermions, $\chi(q, \omega = 0) = \frac{1}{2N} \int_0^\beta d\tau \sum_{i,j} e^{i(q \cdot r_{ij})} (n_{i,c}^\uparrow - n_{i,c}^\downarrow)(\tau)(n_{j,c}^\uparrow - n_{j,c}^\downarrow)(0)$. This quantity is gauge-neutral and demonstrates the magnetic response of the system (note that $\chi$ is also the magnetic susceptibility of the $f$-fermions, as $c$ is related to $f$ by $c_{i\alpha} = f_{i\alpha} S^z_i$, and $(S^z_i)^2 = +1$.) It is interesting to see that in both cases the magnetic responses are strongest in the vicinity of $(\pi, \pi)$ (see the ring-shaped circles) which means that both cases acquire similar shape of FS that gives rise to similar magnetic response, only that in the former it is of the gauge-dependent, hidden FS of $f$-fermions but in the latter, it is the FS of gauge-neutral $c$-fermions.

To make the constrast clearer, in Fig. 1 (c) and (f)
we also prepared the magnetic susceptibility for free fermions. In Fig. 1 (c) we compute the $\chi(q, \omega = 0)$ for doped Dirac fermions, which is generated by the $\pi$-flux square lattice by using $H_f$ in Eq. (1) only and replace the $Z_2$ gauge-field therein with static phase factor $e^{i\phi}$. At the filling $n = 1.13$ we observe almost identical $\chi(q, \omega = 0)$ with that of the Fig. 1 (b), this again implies that the Fermi arc state actually acquires a hidden Fermi pockets of $f$-fermions with the same shape of doped Dirac cones. And consequently gives rise to the same magnetic response as that of the doped Dirac cones, although the actual FS of doped orthogonal semi-metal is the broken Fermi arcs which violate the LT.

Lastly, in Fig. 1 (f), we plot the magnetic susceptibility of free fermion with large FS, obtained from Hamiltonian $H = -\sum_{i,j} (t_{i,j,\alpha} f_{i,\alpha}^\dagger f_{j,\alpha} + h.c.) - \mu \sum_{i} f_{i,\alpha}^\dagger f_{i,\alpha}$, we tune the hopping $t_{i,j}$ with $t_{NN} = 1.0$ and $t_{NNN} = 0.1$ and $\mu = -0.5$ such that this free system will also gives rise to FS similar to Fig. 1 (d). The $\chi(q, \omega = 0)$ of such large FS are shown and it also demonstrate the bright response close to $(\pi, \pi)$.

**PHASE DIAGRAM**

With the Fermi arc and large FS phases seen, we move on to the entire phase diagram. As shown in Fig. 2 (a), our model is the doped version of the orthogonal semi-metal model [42] and when comparing with our previous orthogonal metal model [43], it is the $c$-fermion hopping $t$ that has been added here. And the obtained phase diagram from the QMC simulation, as shown in Fig. 2 (b), contains three different phases: the Fermi arc metal phase, the deconfined FL metal phase and the confined FL metal phase. The transition between Fermi arc and deconfined FL phases is triggered by the composite fermion hopping $t$, as shown in the Fig. 1 (a) and (d) with $t = 0.2$ and $t = 1$, respectively. The heuristic understanding of the FS of these two phases are shown in Fig. 2 (c) and (d). It is clear that inside the Fermi arc phase, the $f$-fermion acquires the FS of doped Dirac cones, as denoted by the light red pockets in Fig. 2 (c), but the FS of the $c$-fermion here is only the broken arcs, as denoted by the solid blue arcs. However, when the $c$-fermion hopping is enhanced, the system enters a metallic phase with large FS, as denoted by the solid blue circle in Fig. 2 (d). Inside this phase, the $Z_2$ gauge field is still deconfined, coexisting with a free fermion metal with large FS.

There is another phase when the $Z_2$ gauge field is confined, with the enhancement of $g$ in $H_g$, this is the confined FL phase in the phase diagram. Here the $Z_2$ gauge field is Higgsed and the phase corresponds to the normal metal phase in our previous orthogonal metal work [43]. The transition from Fermi arc phase and deconfined FL phase to the confined FL phase can be seen from the the average $Z_2$ flux per plaquette, $B = \frac{1}{N} \sum_{\Box} \prod_{k \in \Box} \sigma_5^k$.

and its susceptibility, $\partial (B)/\partial g$, which were used to detect deconfinement-confinement transition [42, 45, 46]. Fig. 3 (a) and (b) show the results in sample paths as $g$ increases. There indeed exist a change in $(B)$ and a peak in $\partial (B)/\partial g$ for $t = 0.3$ in Fig. 3 (a), and for $t = 1.0$ in Fig. 3 (b). These results signify the transition from Fermi arc state with $Z_2$ deconfinement to the confined FL state at $g_c \sim 0.75$ and the transition from deconfined FL state to the confined FL state at $g_c \sim 0.75$. The corresponding phase boundaries in Fig. 2 (b) are drawn in this way.

Fig. 3 (c) tries to locate the Fermi arc to the deconfined FL transition, via the quasiparticle fraction $Z(k) \sim \beta G(k, \beta/2)$ and we chose the antinodal point $k = (\frac{4\pi}{5}, 0)$ with $g = 0.5$ as a function of $t$. It is clear that inside the Fermi arc phase, the quasiparticle fraction is vanishingly small at this finite size ($L = 20$) which hints the existence of gapped spectra there and only Fermi arc remains, while when $t \sim 0.5$ there is a changes of the slope of inceasement of the $Z(k)$ at the antinodal point which suggests the formation of the large FS, although the topological order still persists as shown in Fig. 3 (b). The transition, between the Fermi arc phase and the deconfined FL, is estimated in this way.

FIG. 3. $Z_2$ flux, susceptibility and quasi-particle weight. (a) $t = 0.3, \mu = 1.2, L = 20, T = 0.1$ by tuning $g$, the model goes from Fermi arc phase to confined FL phase. The transition point can be estimated from the peak of the $Z_2$ flux susceptibility $\partial (B)/\partial g$. (b) $t = 1.0, \mu = 1.2, L = 20, T = 0.1$ the transition from deconfined FL phase to confined FL phase can also determined from the $Z_2$ flux and susceptibility data. (c) $g = 0.5, \mu = 1.2, L = 20, T = 0.1$. In order to distinguish the Fermi arc state from the deconfined FL, we monitor the quasi-particle weight $Z(k = (\frac{4\pi}{5}, 0))$ at the antinodal point. In the Fermi arc phase, the antinodal direction is gapped with small weight and in the deconfined FL phase the large FS is formed with substantial weight at antinodal point, one can roughly determine the transition point to be near $t \sim 0.5$. 


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Finally, let’s go back to the Fermi arc phase and clarify a few important points. The first one is whether the FS is indeed broken close to the zone boundary inside the Fermi arc phase, and this can be confirmed from the comparison of the quasiparticle fraction along the nodal and antinodal directions. As shown in Fig. 4, it is clear that at finite temperature, inside the Fermi arc phase, the quasiparticle fraction along the antinodal direction (red triangles) is vanishingly small compared with that along the nodal direction (red circles). Suggesting the existence of pseudogap-like Fermi arc. And inside the deconfined FL phase, the quasiparticle fraction at both directions (black triangles and circles) are well finite, suggesting the existence of a large FS.

Another question is about the properties at the ground state. As shown in Fig. 4, as temperature decreases, the finite quasiparticle fraction at the nodal direction inside the Fermi arc phase also slowly extrapolates to zero (we stress that this is a very rough estimation with only one system sizes and only decreasing the temperature), suggesting the true ground state of the Fermi arc phase is an orthogonal metal with hidden $f$-fermion pockets.

This understanding of the ground state is consistent with the mean-field-theory analysis presented in the SM [44]. In fact, in the limit of $g,t \to 0$, the fluctuation of the $Z_2$ gauge field and the interaction between the $f$-fermions and the Ising spins $S_i^z$ can be ignored, and the system is described by the mean-field picture. In this limit, the $c$-fermion spectrum is given by a convolution of spectra of $f$-fermion and $S^z$ excitations. At finite temperatures, our mean-field calculation indeed shows that this convolution gives Fermi arcs qualitatively similar to the observation of DQMC simulations in Fig. 1(a).

On the other hand, at zero temperature, the $f$-fermion spectrum vanishes because the $S^z$ excitations is gapped (the transverse-field Ising model is in the paramagnetic phase).

With such understanding, we cannot resist the temptation of making connections of our observations with the Fermi arc observed in cuprate experiments [21–26]: our Fermi arc phase shows a strong depletion in the quasiparticle weight at antinodal points (a strong concentration of spectral weight at the nodal points); there is no translational symmetry breaking and the state appears to violate the LT; and the large and closed FS emerges as the hopping of gauge-neutral $c$-fermions increases, resembling of the phenomena in the cuprates near optimal doping.

DISCUSSION

In this work, by means of doping the orthogonal semimetal, we are able to demonstrate a finite-temperature Fermi arc state at generic filling in a lattice model of correlated electrons with unbiased large-scale QMC simulations. The state of Fermi arc can indeed happen without any symmetry-breaking, and therefore appears to violate the Luttinger theorem. We note our state is different from the FL* phase which has a closed Fermi surface, enclosing an area that is different from the prediction of the LT by half BZ, with the other half taken by fractionalized excitations. At the phenomenological level, our Fermi arc state is consistent with the experimental signatures of Fermi surface reconstruction in cuprate materials in the underdoped regime, and its transitions to deconfined and confined FL with large FS, and to other strongly correlated electronic state such as superconductivity are now ready to be explored.

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[43] C. Chen, X. Y. Xu, Y. Qi, and Z. Y. Meng, Chinese Physics Letters 37, 047103 (2020).
[44] QMC implementation of the model, in particular the block update scheme for the $H_c$ term, Mean-field calculation of the spectral properties of the doped orthogonal semi-metal phase, are presented in this Supplemental Material.
SUPPLEMENTAL MATERIAL

QUANTUM MONTE CARLO IMPLEMENTATION

In this supplemental material, we discuss how the quantum Monte Carlo simulation of the model in Eq. (1) is implemented, while part of this introduction is given in our previous orthogonal metal work [43], the addition of the composite fermion hopping term $H_c$ has greatly increased the complexity of Monte Carlo simulations, and we have managed to maintain the similar level of the numerical stability with the block update scheme. We will first recap the construction of the partition function and then pay more attention to the update scheme of $H_c$ term.

After discretizing the imaginary time $\beta = \Delta \tau L_r$, and performing the trace of Ising matter field in the $S^z$ basis, the trace of $Z_2$ gauge field in the $\sigma^z$ basis, and the trace of fermion degrees of freedom to obtain the fermion determinant, the partition function of our model in Eq. (1) can be written as

$$Z = \text{Tr} \{ e^{-\beta H} \}$$

$$= \sum_{\{S_i^z, \sigma_i^z\}} \exp \left[ \sum_{(i,\langle i,j \rangle)} \Delta \tau J S_i^z(l) \sigma_i^z(l) S_j^z(l) + \sum_{i,\langle i,l'\rangle} \gamma_s S_i^z(l) S_i^z(l') \right] \times \exp \left[ \sum_{l,\square} \Delta \tau K b_b^z(l) + \sum_{b,\langle l,l'\rangle} \gamma_B b_b^z(l) b_b^z(l') \right] \times \left| \det \left( I + \prod_{l=1}^{L_r} B(l) \right) \right|^2,$$

where $\gamma_s = -\frac{1}{\beta} \ln \left( \tanh(\Delta \tau h) \right)$, $\gamma_B = -\frac{1}{\beta} \ln \left( \tanh(\Delta \tau g) \right)$, and matrices $B(l) = \exp \left( V(l) \right)$ with $V(l)$ (imaginary time-slice index $l$) takes values $1, \cdots, L_r$, the spatial site index $i, j$ take the values $1, \cdots, L^2$ having elements $V(l)_{i,j} = \Delta \tau \sigma_i^z(l)$ and $V(l)_{i,i} = \Delta \tau \mu$, we will leave the discussion of the $H_c$ term inside $B(l)$ in the next section. The square outside of the determinant comes from two species of fermion (spin up and down). As the bosonic parts of weights are always positive, and the fermion part of weight is a square of determinant of real matrix, the whole weight will be always semi-positive, and it is absence of sign problem.

We therefore perform determinant quantum Monte Carlo to simulate this model, which has been widely used in simulating fermion boson coupled lattice models and more details can be found in the recent review in Ref. [47]. The local updates are performed on the Ising matter field $\{S_i^z\}$ and $Z_2$ gauge fields $\{\sigma_i^z\}$ in a space-time configurational space with volume $L \times L \times L_r$, where $L_r = \beta / \Delta \tau$ with $\Delta \tau = 0.1$ and $\beta = L = 12, 14, \cdots, 20, 24$.

Scheme to update $H_c$ term

$H_c$ is the hopping of the composite $c$-fermion as a combination of orthogonal fermion $f_{i,\alpha}$ and spin matter field $S_i^z$. After the path integral of the partition function, it is equivalent to view the spin variable $S_i^z = \pm 1$ entering the hopping matrix of $f$-fermion.

$$H_c = -t \sum_{(i,\langle j \rangle)} f_{i,\alpha}^\dagger S_i^z f_{j,\alpha} S_j^z + \text{h.c.}$$

Using Trotter decomposition, we can write the $B$ matrix in the fermion determinant in the following form

$$B^\tau = e^{-\Delta \tau T_{\sigma},\tau} \cdot e^{-\Delta \tau T_{\mu},\tau} \cdot e^{-\Delta \tau T_{S^z},\tau}$$

where $T_{\sigma}$ is the matrix from $H_f$ term, $T_{\mu}$ is the chemical potential matrix. And the $T_{S^z}$ is the matrix $T_{S^z,ij} = S_i^z S_j^z$. As shown in Fig. 5, we can further exploit the Trotter decomposition to split the $T_{S^z}$ matrix into A/B sublattice.
FIG. 5. Blue and red dots stand for the $A/B$ sublattice of $S_i^z$ and the cross originated from the blue and red dots are the 4 nearest neighbor (NN) interactions of $S_i^z S_j^z$.

\[ e^{-\Delta \tau T_{S_i^z,A}^{\tau}} = e^{-\Delta \tau T_{S_i^z,A_1}^{\tau}} \cdots e^{-\Delta \tau T_{S_i^z,A_{N/2}}^{\tau}} + \mathcal{O}(\Delta \tau^2) \]
\[ e^{-\Delta \tau T_{S_i^z,B}^{\tau}} = e^{-\Delta \tau T_{S_i^z,B_1}^{\tau}} \cdots e^{-\Delta \tau T_{S_i^z,B_{N/2}}^{\tau}} + \mathcal{O}(\Delta \tau^2) \]

where $N = L^2$ is the number of sites, $A/B$ stands for the elements between $A_i/B_i$ site and its 4 neighboring sites. Matrix $T_{S_i^z,A_i/B_i}$ is zero except for the entries connected by site $A_i/B_i$ and its 4 neighboring sites, illustrated in Fig. 5 for the Eq. 5 type decomposition.

Unlike the DQMC for Hubbard model, where in order to calculate the ratio of determinants and update Green’s function only one element of HS field matrix is involved. We have 4 elements changed when update one $S_i^z$ in $c$-fermion hopping term $H_c$. Now we discuss how to calculate the ratio and update the Green’s function with multiple change of matrix elements. Firstly introduce the $\Delta$ matrix

\[ e^{-\Delta \tau T_{S_i^z,A_i}^{\tau}} = (1 + \Delta) e^{-\Delta \tau T_{S_i^z,A_i}^{\tau}} \]
\[ e^{-\Delta \tau 2 T_{S_i^z,A_i}^{\tau}} = (1 + \Delta) \]

Since once we propose an update $S_i^z \rightarrow -S_i^z$, $T_{S_i^z,A_i}^{\tau} = -T_{S_i^z,A_i}^{\tau}$. One lattice site has four nearest-neighbor hopping so we totally have $2^4 = 16$ $\Delta$ matrices. We can compute all of them in advance to avoid repeatedly calculating them during the simulation.

Below is the general scheme to calculate the ratio and update the Green’s function with $k$ dimensional $\Delta$ matrix [48].

Define

\[ B^M \cdots B^{\tau+1} \equiv B(\beta, \tau) \]
\[ B^{\tau} \cdots B^1 \equiv B(\tau, 0) \]

Try to flip $s_i, \tau$,

\[ \det(1 + B(\beta, \tau)B(\tau, 0)) \rightarrow \det(1 + B(\beta, \tau)(1 + \Delta)(B(\tau, 0))) \]
The weight ratio is
\[
\frac{\det (1 + B(\beta, \tau)(1 + \Delta)(B(\tau, 0)))}{\det (1 + B(\beta, \tau)B(\tau, 0))}
= \det [1 + \Delta (1 - (1 + B(\tau, 0)B(\beta, \tau))^{-1})]
= \det [1 + \Delta (1 - G(\tau, \tau))]
\]
\quad (11)

If update is accepted, we also need update Greens' function
\[
G'(\tau, \tau) = [1 + (1 + \Delta) B(\tau, 0)B(\beta, \tau)]^{-1}
= [1 + B(\tau, 0)B(\beta, \tau)]^{-1}
\left[(1 + (1 + \Delta) B(\tau, 0)B(\beta, \tau)) \left((1 + B(\tau, 0)B(\beta, \tau))^{-1}\right)\right]^{-1}
\quad (12)
\]

As we have \( G \equiv G(\tau, \tau) = [1 + B(\tau, 0)B(\beta, \tau)]^{-1} \), we also denote \( A \equiv B(\tau, 0)B(\beta, \tau) \equiv G^{-1} - I \), then we have
\[
G'(\tau, \tau) = G \left[(1 + (1 + \Delta) A) G^{-1}\right]^{-1}
= G \left[(1 + (1 + \Delta)(G^{-1} - 1)) G\right]^{-1}
= G \left[1 + \Delta (1 - G)\right]^{-1}
\quad (13)
\]

Note \( \Delta (1 - G) \) only have \( k \) rows are none zero, thus can be formulated as the cross product of two rectangular matrix, \( \Delta (1 - G) \equiv UV \), with
\[
U = \begin{bmatrix}
0 & 0 & \cdots \\
\vdots & \vdots & \ddots \\
\Delta_{ii} & \Delta_{ij} & \cdots \\
\vdots & \vdots & \ddots \\
\Delta_{ji} & \Delta_{jj} & \cdots \\
0 & 0 & \cdots \\
\vdots & \vdots & \ddots \\
0 & 0 & \cdots \\
\end{bmatrix}_{N \times k}
\quad (14)
\]

and
\[
V = -\begin{bmatrix}
G_{i1} & \cdots & G_{ii} - 1 & \cdots & G_{ij} & \cdots & \cdots & G_{iN} \\
G_{j1} & \cdots & G_{ji} & \cdots & G_{jj} - 1 & \cdots & \cdots & G_{jN} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots \\
\end{bmatrix}_{k \times N}
\quad (15)
\]

Then with the help of generalized Sherman-Morrison formula \( (I + UV)^{-1} = I - U(I_k + VU)^{-1}V \), we have
\[
G'(\tau, \tau) = G \left[1 + \Delta (1 - G)\right]^{-1}
= G \left((1 + UV)^{-1}\right)
= G \left[I - U(I_k + VU)^{-1}V\right]
= G - GU(I_k + VU)^{-1}V
\quad (16)
\]

Now we try to formulate it in a more standard form (easy extend to delay update). We can factorize \( U \) as
\[
U = \begin{bmatrix}
0 & 0 & \cdots \\
\vdots & \vdots & \ddots \\
\Delta_{ii} & \Delta_{ij} & \cdots \\
\vdots & \vdots & \ddots \\
\Delta_{ji} & \Delta_{jj} & \cdots \\
0 & 0 & \cdots \\
\vdots & \vdots & \ddots \\
0 & 0 & \cdots \\
\end{bmatrix}_{N \times k}
= \begin{bmatrix}
0 & 0 & \cdots \\
\vdots & \vdots & \ddots \\
1_{ii} & 0 & \cdots \\
\vdots & \vdots & \ddots \\
0 & 1_{jj} & \cdots \\
0 & 0 & \cdots \\
\vdots & \vdots & \ddots \\
0 & 0 & \cdots \\
\end{bmatrix}_{N \times k}
\begin{bmatrix}
\Delta_{ii} & \Delta_{ij} & \cdots \\
\vdots & \vdots & \ddots \\
\Delta_{ji} & \Delta_{jj} & \cdots \\
\vdots & \vdots & \ddots \\
\end{bmatrix}_{k \times k}
\equiv \tilde{U}D
\quad (17)
\]
Redefine $U = G \tilde{U}$, $S \equiv D (I_k + \mathbf{VU})^{-1}$, $\mathbf{V} = -\mathbf{V}$, with

$$U \equiv G \tilde{U} = \begin{bmatrix}
G_{11} & G_{12} & \cdots \\
G_{j1} & G_{jj} & \cdots \\
\vdots & \vdots & \ddots \\
G_{N1} & G_{Nj} & \cdots 
\end{bmatrix}_{N \times k}$$

(18)

$$S \equiv D (I_k + \mathbf{VU})^{-1}$$

$$= \begin{bmatrix}
\Delta_{ij} & \Delta_{ij} & \cdots \\
\Delta_{ji} & \Delta_{jj} & \cdots \\
\vdots & \vdots & \ddots \\
\Delta_{Ni} & \Delta_{Nj} & \cdots 
\end{bmatrix}_{k \times k} \begin{bmatrix}
G_{11} & \cdots & G_{i,i-1} & \cdots & G_{ij} & \cdots & \cdots & G_{i,N} \\
G_{j1} & \cdots & G_{ji} & \cdots & G_{jj,i-1} & \cdots & \cdots & G_{jN} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\Delta_{ii} & \cdots & \Delta_{ij} & \cdots & \Delta_{ji} & \cdots & \cdots & \Delta_{nn} \\
0 & \cdots & 0 & \cdots & 0 & \cdots & \cdots & 0 
\end{bmatrix}_{k \times N}^{-1}$$

(19)

and

$$\mathbf{V} \equiv -\mathbf{V} = \begin{bmatrix}
G_{11} & \cdots & G_{i,i-1} & \cdots & G_{ij} & \cdots & \cdots & G_{i,N} \\
G_{j1} & \cdots & G_{ji} & \cdots & G_{jj,i-1} & \cdots & \cdots & G_{jN} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & 0 & \cdots & 0 & \cdots & \cdots & 0 
\end{bmatrix}_{k \times N}$$

(20)

Then we have weight ratio $r = \det(I_k + \mathbf{VU})$ and

$$G'(\tau, \tau) = G + USV$$

(22)

Back to our partition function in Eq. (2) and the update of $H_c$ term, as discussed in the beginning of this section, we have $k = 5$ for updating $S_z^r$. Because we use either Eq. (5) or Eq. (6) to calculate the determinant, we can only update half of $S_z^r$ in one Monte Carlo sweep (in the usual sense). So our scheme is to perform one sweep to try to update $A$ sublattice with Green’s function calculated using Eq. (5) and re-calculate Green’s function using Eq. (6), then update all $B$ sublattice sites. One ‘sweep’ therefore contains two usual sweeps.

**MEAN FIELD CALCULATION OF THE DOPED OSM PHASE**

In this section, we present a mean-field calculation of the spectral properties in the Fermi arc phase of our phase diagram. The calculation here is an extension to the doping case of that for the orthogonal semi-metal case in Ref. [42].

We consider the limit of $g = t = 0$ and neglect gauge field fluctuations and $c$-fermion hopping terms. Since the $c$-fermion spectral function we calculate is a gauge-invariant quantity, we can choose a gauge condition which is $\sigma_{r,\hat{e}} = (-1)^{\tau_x}$ and $\sigma_{r,\hat{y}} = 1$. The $f$-fermion ($\tau_z$ field) is a free fermion (scalar field) hopping in the background of the static gauge field, respectively. So we take the mean-field Hamiltonian

$$\mathcal{H}_f^{MF} = -\sum_{r,\eta} t_{r,\eta} f_{r,\alpha}^\dagger f_{r+\eta,\alpha} - \mu \sum_{r} f_{r,\alpha}^\dagger f_{r,\alpha}$$

(23)

$$\mathcal{H}_\phi^{MF} = \sum_r \frac{1}{2} \omega_r^2 + \frac{1}{2} \sum_{r,\eta} (\Delta_{rr} \phi_r^2 + \sum_{r,\eta} (\phi_r - t_{r,\eta} \phi_{r+\eta})^2)$$

(24)
where $\phi_r$ is a real scalar field and $\pi_r$ is its canonical momentum. $\eta$ takes value in $\{\pm \hat{x}, \pm \hat{y}\}$ and the hopping amplitude $t_{r,\eta} = (-1)^{r+1} \delta_{\eta,\pm \hat{x}} + \delta_{\eta,\pm \hat{y}}$.

The gauge condition breaks the translation symmetry, so momentum space of the mean-field Hamiltonian is defined on a reduced Brillouin zone ($0 < k_x < 2\pi, 0 < k_y < \pi$). For $f$-fermion, substituting $f_{r,\alpha} = \frac{1}{\sqrt{N}} \sum_k f_{k,\alpha} e^{ikr}$

$$H^{MF} = -\sum_{k,k'} f_{k,\alpha}^\dagger f_{k',\alpha} \left( \sum_\eta e^{ik\eta'q} \left( \delta_{\eta,\pm \hat{x}} \delta_{k,k'+\pi k_y} + \delta_{\eta,\pm \hat{y}} \delta_{k,k'} \right) + \mu \delta_{k,k'} \right)$$

$$= -\sum_k 2 \cos(k_x) f_{k,\alpha}^\dagger f_{k+\pi k_y,\alpha} + (2 \cos(k_y) + \mu) f_{k,\alpha}^\dagger f_{k,\alpha}$$

$$= -\sum_k' \left( f_{0,\alpha}(k) \right) \left( \begin{array}{cc} 2 \cos(k_y) + \mu & 2 \cos(k_x) \\ 2 \cos(k_x) & -2 \cos(k_y) + \mu \end{array} \right) \left( f_{0,\alpha}(k) \right)$$

where $f_{0,\alpha}(k) = f_{k,\alpha}, f_{\pi,\alpha}(k) = f_{k+\pi k_y,\alpha}$ and $\sum'$ is the sum of momentum in the reduced Brillouin zone. Diagonalizing the Hamiltonian, we get the energy spectrum $\epsilon_{\pm}(k)$ and the eigen-modes $f_{\rho,\gamma}(k) = V_{\rho,\gamma}(k) f_{\gamma,\alpha}(k)$, where $\gamma = \pm, \rho = 0/\pi$ and $V_{\rho,\gamma}$ diagonalize the Hamiltonian. It is useful to represent $f_{k,\alpha}$ by $f_{\gamma,\alpha}(k)$

$$f_{k,\alpha} = V_{\rho(k),\gamma}(P(k)) f_{\gamma,\alpha}(P(k)) \quad, \quad \rho(k) = \begin{cases} 0, & k_y \in [0,\pi) \\ \pi, & k_y \in [\pi,2\pi) \end{cases} \quad, \quad P(k) = \begin{cases} k_y, & k_y \in [0,\pi) \\ k_y - \pi, & k_y \in [\pi,2\pi) \end{cases}$$

$f$-fermion spectrum function is (it is equivalent to understand $A_f(k,k',\omega)$ as $A_f(k,\omega)_{\rho,\rho'}$. Momentum of the later one is in reduced BZ.)

$$A_f(k,k',\omega) = \frac{1}{2\pi} \int dt e^{i\omega t} \left\langle \{ f_k(t), f_{k'}^\dagger \} \right\rangle$$

$$= \sum_{\gamma} \delta(\omega - \epsilon_{\gamma}(P(k))) \delta_{P(k),P(k')} V_{\rho(k),\gamma}(P(k)) V_{\rho(k'),\gamma}(P(k))$$

FIG. 6. Mean-field $c$-fermion spectral function $A(k,\omega = 0)$. The parameters are $L = 20, T = 0.1, \mu = 1.2, \omega = 1$ and $\Delta = -1.1$. 
For scalar field, substituting $\phi_r = \frac{1}{\sqrt{N}} \sum_k \phi_r e^{ikr}$

$$\mathcal{H}_{\phi}^{MF} = \sum_k \frac{1}{2} \pi_k \pi_k + \frac{1}{2} m \omega^2 \left( \Delta \phi_k \phi_{-k} + (4 - 2 \cos(k_y)) \phi_k \phi_{-k} - (2 \cos(k_x)) \phi_k \phi_{-k} \pi_{k_y} \right)$$

$$= \sum_{k, \rho} \frac{1}{2} \pi_k \pi_{-k, \rho} + \sum_k \frac{1}{2} \omega^2 \left( \phi_0(k) \phi_0(k) \right) \left( \Delta + 4 - 2 \cos(k_y) \right) \left( -2 \cos(k_x) \right) \left( \Delta + 4 + 2 \cos(k_y) \right) \left( \phi_0(-k) \phi_0(-k) \right)$$

Diagonalizing the frequency matrix, we get the eigen-frequency $\omega_\kappa(k)$ and the normal modes $\phi_\kappa(k) = U_\kappa(k) \phi_\kappa(k)$ (caution: the eigenvalue of the matrix is the square of $\omega_\kappa(k)$, so we must set $\Delta > 2 \sqrt{2} - 4$, otherwise the eigenvalue will be negative.). To diagonalize the Hamiltonian, we introduce operators

$$\begin{align*}
a_\kappa(k) &= \sqrt{\frac{1}{2} \omega_\kappa(k)} \phi_\kappa(k) + i \sqrt{\frac{1}{2 \omega_\kappa(k)}} \pi_\kappa(k) \\
a_\kappa(k)^\dagger &= \sqrt{\frac{1}{2} \omega_\kappa(k)} \phi_\kappa(k) - i \sqrt{\frac{1}{2 \omega_\kappa(k)}} \pi_\kappa(k)
\end{align*}$$

then the Hamiltonian becomes

$$\mathcal{H}_{\phi}^{MF} = \sum_{k, \kappa} \omega_\kappa(k) a_\kappa(k) a_\kappa(k) + \text{const.}$$

Representing $\phi_k$ by $a$ and $a^\dagger$

$$\phi_k = \frac{U_\kappa(k) \pi(k)}{\sqrt{2 \omega_\kappa(k)}} \left( a_\kappa(P(k)) + a_\kappa^\dagger(-P(k)) \right)$$

There is some subtlety in the commutation relation. Notice that $\phi_0(-k)(\phi_\kappa(-k))$ is defined as $\phi_{-k}(\phi_{k-\pi k_y})$, we will get a strange commutation relation between positive $k_y$ and negative $k_y$. In the calculation of Hamiltonian, we don’t meet any problem because the commutation relation have the same momentum, but that’s not the case in the calculation of spectrum function. At least, we can require $k, k' > 0$ to avoid the subtlety.

$$A_\phi(k, k', \omega) = \frac{1}{2 \pi} \int dte^{i\omega t} \langle [\phi_k(t), \phi_{-k'}] \rangle$$

$$= \frac{1}{2 \pi} \int dte^{i\omega t} \sum_{\kappa, \kappa'} U_\rho(k, \kappa) U_\rho(-k', \kappa') \left( \frac{1}{\sqrt{4 \omega_\kappa(P(k)) \omega_{\kappa'}(-P(k'))}} \right) \times \left( \langle a_\kappa(P(k)) + a_\kappa^\dagger(-P(k)) \rangle + \langle a_\kappa(-P(k)) + a_\kappa^\dagger(-P(k)) \rangle \right)$$

$$= \sum_{\kappa} \left[ \delta(\omega - \omega_\kappa(P(k))) - \delta(\omega + \omega_\kappa(P(k))) \right] \delta P(k), -P(k') \times \frac{1}{\sqrt{4 \omega_\kappa(P(k)) \omega_{\kappa'}(-P(k))}}$$

Finally, we calculate the Matsubara Green’s function $\mathcal{G}(k, k', \omega_n) = \int d\omega A_{k, k', \omega_n}$, and convolute fermion and scalar field Green’s function to obtain c-fermion Green’s function, note that c-fermion Green’s function is gauge invariant, so we can simply set $k = k'$.
The last step is a Matsubara sum which is calculated by the standard way. As an example, the $c$-fermion spectral function from finite size mean-field calculation, with the same temperature and filling compared with that in the QMC simulation inside the Fermi arc phase, is given in Fig. 6.