Fractionalized Metal in a Falicov-Kimball Model

Martin Hohenadler and Fakher F. Assaad
Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany
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Quantum Monte Carlo simulations reveal an exotic metallic phase with a single-particle gap but gapless spin and charge excitations and a non-saturating resistivity in a two-dimensional SU(2) Falicov-Kimball model. An exact duality between this model and an unconstrained slave-spin theory leads to a classification of the phase as a fractionalized or orthogonal metal whose low-energy excitations have different quantum numbers than the original electrons. Whereas the fractionalized metal corresponds to the disordered regime of the slave spins, the ordered regime is a Fermi liquid. At a critical temperature, we observe an Ising phase transition to a spontaneously generated constrained slave-spin theory of the Hubbard model.

The fractionalization of electrons into objects with new quantum numbers is among the most fascinating consequences of strong interactions. It is ubiquitous in one-dimensional (1D) metals, where Fermi liquid theory breaks down completely and the low-energy properties are instead determined by collective charge and spin excitations [1]. Fractionalization is less common but physically even richer in higher dimensions, where it involves emergent degrees of freedom such as spinons or gauge fields [2]. A prime example are genuine Mott insulators without magnetic order that can be classified as topologically ordered quantum spin liquids [3, 4]. Experiments on, for example, high-temperature superconductors also reveal strange metallic states at higher temperatures such as non-Fermi liquids [5] or bad metals [6], which are believed to be strongly tied to the exotic low-temperature physics. In orthogonal metals [2], with Fermi-liquid-like transport and thermodynamics but no quasiparticles, non-Fermi-liquid physics arises from fractionalization and reconciles the absence of quasiparticles in photoemission with a Fermi surface according to quantum oscillation measurements [7]. Finally, unusual metallic states have become a focus of applications of the gauge/gravity duality [8, 10].

Recent insights into fractionalized phases have in particular come from exactly solvable models [7, 10, 11] and designer Hamiltonians suitable for quantum Monte Carlo (QMC) simulations [12, 14]. However, the corresponding models have only limited overlap with the standard models of condensed matter theory. Among the latter, the Hubbard model [15] continues to attract interest [16–18], to a significant part due to its expected relevance for high-temperature superconductivity. The Falicov-Kimball model (FKM) [19] is significantly simpler because electrons of one spin sector remain localized [15]. It admits an exact solution in infinite dimensions where it exhibits a quantum phase transition [20], as well as exact mathematical theorems [21]. FKMs are also instrumental to understand correlated electrons out of equilibrium [22]. While traditionally not associated with the intricate physics of fractionalization, they have recently emerged in the context of lattice gauge theories [23, 24]. Finally, FKMs of spinless fermions have recently been shown to exhibit localization without disorder [25].

In this Letter, we show that a fractionalized metallic phase emerges in quantum Monte Carlo (QMC) simulations of a simple 2D FKM. This model has no exact solution, but instead reduces to the Hubbard model at $T = 0$ and/or in infinite dimensions. The observed physics can be understood by exploiting an exact relation to an unconstrained Ising lattice gauge theory via a slave-spin representation. Mean-field arguments reveal the basic mechanism for fractionalization, whereas our simulations fully account for quantum and thermal fluctuations to establish the existence of such a phase in this model.

Model.—We consider the Hamiltonian

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} (c_{i \sigma}^\dagger c_{j \sigma} + \text{H.c.}) - U \sum_{i} \hat{Q}_{i} \prod_{\sigma} (\hat{n}_{i \sigma} - \frac{1}{2}). \tag{1}$$

Here, $c_{i \sigma}^\dagger$ creates a spin-$\sigma$ electron at site $i$ of a square lattice and $\hat{n}_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma}$. The first term describes nearest-neighbor hopping. Restricting $\sigma$ to a single value yields a standard FKM [19] with the localized fermions expressed in terms of the Ising degrees of freedom $Q_i = \pm 1$ via the relation $\hat{n}_{i \sigma}^{\text{loc}} = (Q_i - 1)/2$. For two flavors $\sigma = \uparrow, \downarrow$, the second term in Eq. (1) becomes a three-body interaction of the Hubbard-Ising form $U \sum_i Q_i (\hat{n}_{i \uparrow} - \frac{1}{2})(\hat{n}_{i \downarrow} - \frac{1}{2})$. Generalizations to SU($N$) fermions with $N > 2$ flavors or higher-spin $Q_i$ variables are also conceivable. For $N > 1$, the product over flavors renders Eq. (1) not exactly solvable even in infinite dimensions; we consider $N = 2$ in the following. The Ising variables $\hat{Q}_i$ are locally conserved, $[\hat{H}, \hat{Q}_i] = 0$. At the particle-hole symmetric point investigated here, Hamiltonian (1) has an O(4) = SO(4) × Z$_2$ symmetry. The SO(4) symmetry is the same as for the Hubbard model [26]. The global Z$_2$ symmetry reflects invariance under $Q_i \to -Q_i$ in combination with a particle-hole transformation [27] that yields $U \to -U$; it can be broken at $T > 0$ in the 2D case considered.

We use units in which $k_B = t = 1$ and consider periodic $L \times L$ lattices. Simulations were done using the auxiliary-field QMC method [28] from the Algorithms for Lattice Fermions library [29], see also the SM [30].
**Ising phase transition.**—Similar to other FKMIs [20], in our model, the latter corresponds to a ferromagnetic phase transition of the Ising variables $Q_i$ at a critical temperature $T_Q$ that reduces the symmetry from $O(4)$ to $SO(4)$. Its origin can be traced back to an exchange coupling $J \sum_{ij} Q_i Q_j$—mediated by the itinerant fermions—that is allowed by the symmetries of Eq. 1 and hence generated. The onset of order is visible from the squared magnetization per site $m^2_Q = M^2_Q / L^2$, where $M^2_Q = \frac{1}{L} \sum_j \langle \hat{Q}_i \hat{Q}_j \rangle$, shown in Fig. 1(a). The 2D Ising universality is revealed by the finite-size scaling in Fig. 1(b) with exponents $\beta = 1/8$ and $\nu = 1$. For the phase diagram in Fig. 1(c), we estimated the critical temperature from $m^2_Q(T_Q) = 0.5$ using $L = 8$ and $L = 12$. The dependence of $T_Q$ on $U$ is reminiscent of $T_c$ for the charge-density-wave (CDW) transition of the spinless, half-filled FKM [31, 32]. In particular, $T_Q = 0$ at $U = 0$ due to the absence of exchange interactions, and $T_Q \to 0$ for $U \to \infty$ because $T_Q \sim J \sim t^2 / U$.

Upon replacing the Ising variables $\hat{Q}_i$ by mean-field values $\langle \hat{Q}_i \rangle = 0$ (for $T > T_Q$) or $\langle \hat{Q}_i \rangle = m_Q$ (for $T < T_Q$), the SU(2) FKM of Eq. 1 reduces to free fermions ($T > T_Q$) or a Hubbard model ($T < T_Q$). We have verified that below $T_Q$ we quantitatively recover Hubbard model results for $T \to 0$ [33], namely an antiferromagnetic Mott insulator ($m_Q = -1$) or coexisting CDW order and s-wave superconductivity ($m_Q = +1$), respectively [34].

**Two distinct metallic regimes.**—The novel physics of this Letter occurs at $T > T_Q$, where we find two distinct metallic regimes. A mean-field solution of Eq. 1 with $\langle \hat{Q}_i \rangle = 0$ captures the Fermi liquid observed at weak $U$. The fractionalized metal at large $U$ will naturally emerge from a slave-spin mean-field theory below. The two different metallic regimes indicated in Fig. 1(c) are revealed by the QMC results in Fig. 2. The single-particle spectral function $\mathcal{A}(k, \omega)$ at temperature $T = 1/6$ in (a) the Fermi liquid and (b) the fractionalized metal. (c) Conductivity and (d) resistivity $\rho = 1/\sigma dc$ (inset: logarithmic scales). Here, $L = 8$.
the fractionalized metal has strongly renormalized but
gapless long-wavelength (i.e., \(q \to 0\)) spin excitations, as
visible from the dynamic spin structure factor \(S^s(q, \omega)\)
in Fig. 3(a). These excitations give rise to an in-
crease of the spin susceptibility \(\chi_s = \beta (\langle M^2 \rangle - \langle M \rangle^2)\)
(here, \(M = \sum_i \hat{s}_i^z\)) with decreasing temperature down to
\(T_Q = t/U\), see Fig. 3(b)); this behavior is again beyond
Fermi liquid theory where a single-particle gap implies
\(\chi_s \to 0\) for \(T \to 0\). The results for the attractive Hub-
bard model in Fig. 3(b) instead exhibit an exponential
suppression of \(\chi_s\) below \(T_\star \sim U\) [30]. Because of the
O(4) symmetry at half-filling, the spin structure factor
and the spin susceptibility of the FKM are identical to
their charge counterparts. Hence, Fig. 3 also con-
firms the existence of gapless charge excitations and hence a
metallic state.

**Duality and Fractionalization.**—To connect the dis-
tinct properties observed in the metallic regime at large \(U\)
to fractionalization, we exploit a duality transformation
between the FKM (1) and an unconstrained \(Z_2\) slave-spin
theory. To arrive at the latter, we first relabel the states
of the local Hilbert space from \(|\{0\}_i, \{j\}_i, \{\downarrow\}_i, \{\downarrow\}_i\rangle \otimes
|\{+1\}_j, \{-1\}_j\rangle\) to \(|\{0\}_i, \{\downarrow\}_i, \{\downarrow\}_i, \{\uparrow\}_i\rangle \otimes
|\{1\}_j, \{1\}_j\rangle\). Next, we represent the fermionic
operators by

\[
c_{i\sigma}^{(1)} = f_{i\sigma}^{(1)} s_i^z, \tag{2}\]

and the Ising variables as

\[
\hat{Q}_i = \hat{s}_i^z (-1)^{\sum_x f_{ix} f_{i\sigma}}. \tag{3}\]

Here, \(f_{i\sigma}^{(1)}\) is a fermionic operator and \(\hat{s}_i^z, \hat{s}_i^x\) correspond
to Pauli spin matrices. Using the operator identity
\((-1)^{\sum_x f_{ix} f_{i\sigma}} \equiv (2\hat{n}_{1\uparrow} - 1)(2\hat{n}_{1\downarrow} - 1)\) yields the slave-spin
formulation of the FKM (1),

\[
\hat{H}^{fs} = -t \sum_{\langle ij \rangle \sigma} (f_{i\sigma}^{\dagger} f_{j\sigma} + f_{j\sigma}^{\dagger} f_{i\sigma}) + \frac{U}{4} \sum_i \hat{s}_i^z. \tag{4}\]

Equation (4) locally conserves the \(\hat{Q}_i, [\hat{H}^{fs}, \hat{Q}_i] = 0\),
and corresponds to an unconstrained gauge theory in the
sense that we do not impose the Gauss law corresponding
to \(\hat{Q}_i |\psi\rangle = |\psi\rangle\) or simply \(\hat{Q}_i = 1\). This unconstrained
theory is an exact slave-spin representation of Eq. (1).

Enforcing \(\hat{Q}_i = 1\) amounts to projecting onto the 4D local
Hilbert space of the Hubbard model and promotes
Eq. (4) to an exact (constrained) \(Z_2\) slave-spin theory of
the latter. This also becomes apparent from Eq. (1) upon
setting \(\hat{Q}_i = 1\). An intriguing question is under what con-
ditions the constrained and unconstrained theories are equivalent.

According to Fig. 4 the constraints \(\hat{Q}_i\) are
spontaneously generated in the ferromagnetic phase at
\(T < T_Q\) so that for \(T \to 0\) the unconstrained theory
(1) becomes an exact slave-spin representation of the
Hubbard model. Moreover, the constraints are completely
irrelevant at \(U = 0\) [where both Eq. (1) and Eq. (4) re-
duce to free fermions] and in infinite dimensions for any
\(U\) and \(T\); the latter statement holds only at the particle-
hole symmetric point and was previously proved in the
slave-spin representation [35]. It also follows directly for
the half-filled FKM (1) because the only nonzero con-
tributions in a diagrammatic expansion in the interac-
tions \(U \sum_i \hat{Q}_i (\hat{n}_{1\uparrow} - \frac{1}{2})(\hat{n}_{1\downarrow} - \frac{1}{2})\) contain even numbers of
vertices at a single site (the free propagator is local for
\(D = \infty\) [39, 42] and \(\langle \hat{Q}_i \rangle^{4n} = 1\).

A mean-field theory of the dual slave-spin model (4)
captures the metallic state observed at strong coupling
and relates it to fractionalization. The product
ansatz \(|\Phi\rangle_{MF} = |\phi\rangle_f \otimes |\phi\rangle_s\) for the ground-state de-
couples the problem into a free-fermion part \(\hat{H}_{MF}^{fs} =
- t \sum_{\langle ij \rangle \sigma} g_{ij} (f_{i\sigma}^{\dagger} f_{j\sigma} + f_{j\sigma}^{\dagger} f_{i\sigma})\) and a transverse-field Ising
model \(\hat{H}_{MF}^{is} = - t \sum_{\langle ij \rangle} J_{ij} \hat{s}_i^z \hat{s}_j^z - \frac{\nu}{4} \sum_i \hat{s}_i^z\) connected by the self-consistency conditions \(g_{ij} = \langle \hat{s}_i^z \hat{s}_j^z \rangle_s\) and \(J_{ij} =
\sum_{\sigma} \langle f_{i\sigma}^{\dagger} f_{j\sigma} + H.c. \rangle_f\) [27]. The slave spins will be fer-
magnetically ordered for \(U < U_c\), and disordered for \(U > U_c\).
The effect of this transition on the original
electrons becomes clear from their spectral function,
\(A(k, \omega) = \langle \hat{s}_k^z \rangle^2 \delta(\omega - E_k)\) [7], where \(E_k\) is the free-fermion
dispersion. Clearly, \(\langle \hat{s}_k^z \rangle^2\) is directly related to the quasi-
particle residue \(Z\), which is finite for \(U < U_c\) but vanis-
ishes for \(U > U_c\). Within single-site mean-field theo-
ries, including dynamical mean-field theory, this transi-
tion is associated with a Mott metal-insulator transition
for which \(\langle \hat{s}_k^z \rangle\) serves as an order parameter [37, 11].

Beyond single-site mean-field theories, \(\langle \hat{s}_k^z \rangle^2 \neq \langle \hat{s}_k^x \rangle^2\),
and the disordered phase is an orthogonal metal with Drude
weight \(D \sim \langle \hat{s}_i^z \hat{s}_j^z \rangle\) rather than a Mott insulator [7].

In the context of slave-spin representations, fraction-
alization amounts to the dissociation of the physical c-
electrons into auxiliary f-fermions that carry the phys-
ical U(1) charge [7] and the slave spins \(\hat{s}_i^z\). Whereas the
c-fermions are invariant under local gauge transfor-
mations generated by the \(Q_i\), the f-fermions and slave
spins each carry a \(Z_2\) gauge charge that manifests itself
as \(\hat{Q}_i f_{i\sigma}^{(1)} \hat{Q}_i = - f_{i\sigma}^{(1)}\), \(\hat{Q}_i \hat{s}_i^z \hat{Q}_i = - \hat{s}_i^z\). While this charge is
strictly conserved only in constrained gauge theories, the
notion of fractionalization remains meaningful in a
broader context, including mean-field theories, where the constraints are either ignored or imposed on average \[37\], and unconstrained gauge theories such as Eq. \[4\], where the charge is conserved in space but not in time. In particular, the orthogonal metal emerging in mean-field theory at \(U > U_c\) from the disordering of the slave spins may be regarded as fractionalized in the sense that the metallic properties are carried by the \(Z_2\)-charged \(f\)-fermions that are orthogonal \[7\] to the gauge-invariant \(c\)-fermions.

The mean-field fractionalization scenario is essentially borne out by our QMC results for the FKM: as shown in Fig. 2, the single-particle spectrum has a gap at large \(U\) but the system remains metallic. Within our unbiased QMC approach, the mean-field phase transition of the slave spins is replaced by an order-disorder crossover reflected in the slave-spin correlator \(G^s(\tau) = \langle \hat{s}_i^x(\tau)\hat{s}_i^x \rangle\) in Fig. 4(a), which is directly related to the opening of the single-particle gap visible in Fig. 2. The disorder of the slave spins strongly enhances scattering and suppresses coherent quasiparticle motion \(\text{Fig. 2(c)}\). However, the current-current correlations \(\Gamma_{xx}(q = 0, \tau)\) \[30\] in Fig. 4(b) remain gapless even for large \(U\).

Discussion—While the non-Fermi-liquid regime at large \(U\) exists independent of the slave-spin representation, the latter reveals the fractionalization and close conceptual relations to orthogonal metals \[7\]. On the other hand, our findings differ in a number of important details from previous mean-field and exact realizations of orthogonal metals \[4\]. First, our simulations preserve the local \(Z_2\) gauge symmetry of Eq. \[4\], in accordance with Elitzur’s theorem \[12\]. This symmetry—reflecting invariance under the local transformation \(f_{\sigma \sigma}^{(t)} \rightarrow -f_{\sigma \sigma}^{(t)}, \hat{s}_i^z \rightarrow -\hat{s}_i^z\) generated by \(\hat{Q}_1\)—implies that the spatial correlations \(\langle \hat{s}_i^z \hat{s}_j^z \rangle_{\hat{J}}\) are responsible for a nonzero Drude weight in mean-field theory are zero \[12\]. Accordingly, the slave spins undergo a crossover [in imaginary time, see Fig. \(4\text{a})\)] instead of a phase transition. Similarly, the \(f\)-fermions are localized because they also carry \(Z_2\) charge and the gapped but dispersive single-particle excitations in Fig. \(2\text{b})\) instead emerge from the combination of imaginary-time correlations (i.e., quantum fluctuations) and vertex corrections. If the latter are absent, as in infinite dimensions, a single-particle gap always implies insulating behavior \[39\]. Whereas the orthogonal metals in the exactly solvable models of Ref. \[7\] are non-interacting, transport and thermodynamic properties are strongly renormalized by interactions in the present, correlated fractional metal. Finally, in contrast to the \(t-J\) model with random interaction \[10\], our fractionalized phase arises in a fully translation-invariant setting.

Our work has connections to several other areas of current interest. A 1D unconstrained gauge theory (equivalent to a spinless FKM) was recently shown to exhibit localization without disorder \[25\]. The quantum percolation mechanism in the 2D case \[24\] may be connected to the metallic behavior observed here. The slave-spin formulation \[4\] provides a link to recent simulations of lattice gauge theories coupled to fermions that exhibit exotic phases and phase transitions \[12\] \[44\] as well as Sachdev-Ye-Kitaev models \[10\]. Progress on cold-atom realizations of FKM and Hubbard models \[18\] \[43\] \[44\] as well as lattice gauge theories \[45\] promise the possibility of experimentally observing the fractionalized metal, facilitated by its stability at high temperatures.

In summary, we have presented unbiased numerical evidence for a non-Fermi-liquid phase in a simple 2D Falicov-Kimball model. This Fermi metal differs from phases of incoherently paired fermions (i.e., bosons) such as the paired Fermi liquid known from the attractive Hubbard model, and previous realizations of orthogonal metals. The exact relation to an unconstrained slave-spin representation allowed us to understand the physics in terms of fractionalization of the original electrons.

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Supplemental Material

Methods

Given the exact duality that relates Eqs. (1) and (4), the simulations were carried out in the slave-spin representation. The site Ising variables in Eq. (4) were mapped to bond Ising variables. The resulting Hamiltonian takes the form

$$\hat{H}_0^{\text{IS}} = -t \sum_{\langle ij \rangle \sigma} \langle f_{i \sigma} f_{j \sigma} + \text{H.c.} \rangle \hat{Z}_{ij} - \frac{U}{4} \sum_i \hat{X}_{i+\hat{x}} \hat{X}_{i-\hat{x}} \hat{X}_{i+\hat{y}} \hat{X}_{i-\hat{y}},$$

(5)

where the second term flips all four bond Ising spins attached to site $i$. In this representation, the constraint $\prod_{\langle ij \rangle \in \partial \Box} \hat{Z}_{ij} = 1$ ($\partial \Box$ denotes the bonds of a plaquette) holds and ensures that the number of degrees of freedom remains constant. This constraint was imposed in the simulations.

Simulations were carried out using the auxiliary-field QMC code from the Algorithms for Lattice Fermions (ALF) library [29]. In the present case, the role of the auxiliary fields is taken by the bond Ising variables in Eq. (5). The grand-canonical partition function is written as a Euclidean path integral over Ising spin configurations $Z = \{Z_{ij}\}$,

$$Z = \text{tr} e^{-\beta (H - \mu N)} = \int \mathcal{D}[Z] e^{-S[Z]}.$$

(6)

As usual, imaginary time was discretized with a Trotter timestep $\Delta \tau = \beta / L$ ($\beta = 1 / T$ is the inverse temperature); we used $\Delta \tau U \leq 0.1$. The configuration weight can be written as $e^{-S} = e^{-S_0} \det[1 + B(Z)]$. Here, $S_0$ describes the spin dynamics due to the transverse field in Eq. (5), whereas $B$ is a product over time slices of exponentials of the hopping term that contains the fermion-spin coupling. Because $S$ is real, there is no sign problem. Since each bond spin $\hat{Z}_{ij}$ is related to two site spins $\hat{s}_i^z$ and $\hat{s}_j^z$, the minimal update consists of flipping all four bond spins connected to a site $i$. To make the mapping between site and bond spins bijective, we stored a reference eigenvalue $\hat{s}_i^z_{\text{ref}}$ for each configuration.

Observables were measured using the single-particle Green function and Wick’s theorem [47]. Apart from the gauge-invariant observables defined in terms of the original fermions, we also measured correlation functions of the configuration.

Methods

Here we provide definitions for some of the observables shown in the Letter. The fermionic spin operator is defined as $\hat{S}_i^z = (\hat{n}_{\uparrow i} - \hat{n}_{\downarrow i}) / 2$. The Lehman representation of the dynamic spin structure factor reads

$$S^z(q, \omega) = \frac{1}{Z} \sum_{mn} |\langle m | \hat{S}_q^z | n \rangle|^2 e^{-\beta E_n} \delta(E_n - E_m - \omega),$$

(7)

where $|m\rangle$ is an eigenstate with eigenvalue $E_m$. The current-current correlation function $\Gamma_{xx}(q, \tau)$ is the Fourier-transform of

$$\Gamma_{xx}(r, \tau) = \langle j_x(r, \tau) j_x(0, 0) \rangle$$

(8)

with the current operator $\hat{j}_x(r) = \sum_{\sigma} \langle c_{r+\hat{e}_x, \sigma} \hat{c}_{r, \sigma}^\dagger - \hat{c}_{r, \sigma} \hat{c}_{r+\hat{e}_x, \sigma}^\dagger \rangle$. From $\Gamma_{xx}(q, \tau)$, we extracted the dc conductivity $\sigma_{dc} = \lim_{\omega \to 0} \text{Re} \sigma_{\text{reg}}$ without analytic continuation by using [49]

$$\sigma_{dc} = \frac{\beta^2}{\pi} \Gamma_{xx}(q = 0, \tau = \beta / 2).$$

(9)

Absence of superconductivity

We have directly verified the absence of any signatures of superconducting behavior in the FKM by calculating the superfluid density $D_s = -\epsilon_{\text{kin}, x} - \Gamma_{xx}(q_x = 0, q_y \to 0, \omega = 0)$ where $\epsilon_{\text{kin}, x} = \sum_{\sigma} \langle c_{r}^\dagger \sigma c_{r+\hat{e}_x, \sigma} + \text{H.c.} \rangle$ [50]. It scales to zero for all parameters considered.
Finite-size scaling of the conductivity at $T = 1/6$.

**Finite-size scaling of $\sigma_{dc}$**

To demonstrate that the nonzero conductivity in the fractionalized metallic phase is not a finite-size artifact, Fig. 5 shows a finite-size scaling for different values of $U$. Whereas $\sigma_{dc}$ decreases slightly in the Fermi liquid phase at $U = 4$, it actually increases with increasing $L$ and has a very weak size dependence in the fractionalized phase.