

Towards the standard model for Fermi arcs from a Wilsonian reduction of the Hubbard model

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Two remarkable features emerge from the exact Wilsonian procedure for integrating out the high-energy scale in the Hubbard model. At low energies, the number of excitations that couple minimally to the electromagnetic gauge is less than the conserved charge, thereby implying a breakdown of Fermi liquid theory. In addition, two charge e excitations emerge in the lower band, the standard projected electron and a composite entity (comprised of a hole and a charge $2e$ bosonic field), which give rise to poles and zeros of the single-particle Green function, respectively. The poles generate spectral weight along an arc centered at $(\pi/2, \pi/2)$, while the zeros kill the spectral intensity on the back side of the arc. The result is the Fermi arc structure intrinsic to cuprate phenomenology. The presence of composite excitations also produces a broad incoherent pseudogap feature at the $(\pi, 0)$ region of the Brillouin zone, thereby providing a mechanism for the nodal/antinodal dichotomy seen in the cuprates.

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I. INTRODUCTION

As revealed by extensive angle-resolved photoemission spectroscopy (ARPES) studies,^{1–7} lightly doped copper-oxide superconductors (cuprates) in the pseudogap regime possess a band of excitations that only cross the chemical potential once. Such a single crossing generates a set of coherent or pole-like excitations that ultimately form a truncated Fermi region, termed a Fermi arc, as opposed to the traditional Fermi surface generated by a double crossing. The coherent excitations, centered around $(0, 0) \rightarrow (\pi, \pi)$, traverse the zone diagonal and terminate in the vicinity of $(\pi, 0)$ or $(0, \pi)$, thereby giving rise to a nodal/antinodal dichotomy,^{8–12} the former being ungapped while the latter is gapped. While some ARPES experiments¹³ performed on $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ (La-Bi2201) revealed closed hole pockets, and hence consistency with the results from quantum oscillation experiments in high magnetic fields,^{14–18} this interpretation has been called into question.⁶ King *et al.*⁶ observed that the closed pockets seen earlier¹³ are entirely structural in origin, as they originate from overlapping superstructure replicas of the main and shadow bands. Consequently, the preponderance of evidence from ARPES is that the coherent excitations form a disconnected region in momentum space consistent with a single crossing of the chemical potential.

Theoretically, two questions arise. (i) What suppresses the spectral weight on the back side of the arc? and (ii) What is the origin of the incoherent excitations or gap at the zone boundary? A natural candidate to explain the former is that two kinds of excitations populate a doped Mott insulator, one of which has no overlap with the electron. Such an excitation will appear in the single-electron Green function as a zero rather than a pole and hence will carry no spectral weight. In this vein, some have proposed neutral composite excitations¹⁹ to explain the origin of Fermi arcs. Alternatively, Fermi arcs have been seen in numerics^{20–22} in the two-dimensional Hubbard model and have been modeled phenomenologically²³ (Yang, Rice, and Zhang; hereafter YRZ). However, a key assumption of the phenomenological account is that the zero line is fixed at the diamond-shaped Fermi surface of the noninteracting system. That the diamond-shaped Fermi surface of the noninteracting

system constitutes the zero line of the single-particle Green function is a rigorous mathematical statement²⁴ only if the underlying Hamiltonian is particle-hole symmetric. In fact, from the precise condition^{24–26} for the vanishing of the real part of the Green function, maintaining that the zero line is doping independent requires unphysical assumptions regarding the spectral function. Certainly such a conservation of the zero line is not borne out by numerics on the Hubbard model^{27,28} or by analytical arguments.²⁴ In addition, models involving Cooper pairs, fluctuating or otherwise, have been constructed to yield either arcs⁵ or hole pockets.^{29,30} Our discussion here, however, focuses entirely on arcs, as this seems to be what the ARPES experiments are about.

While the physical origin of arcs might not be clear, the mathematics is. Any Green function of the form

$$G_{\text{toy}}(\omega, \mathbf{k}) = \frac{Z}{\omega - \epsilon_{\mathbf{k}} + \frac{|\Delta(\mathbf{k})|^2}{\omega - \epsilon_{\mathbf{k}}}} \quad (1.1)$$

will do. The similarity to the BCS Green function is only perfunctory, as there is no anomalous component. Aside from having poles, Eq. (1.1) has zeros whenever $\epsilon_{\mathbf{k}} = 0$, assuming of course that the chemical potential corresponds to $\omega = 0$. While the two dispersing electronic bands, $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}}$, in Eq. (1.1) are not hard to come by, the parameter $\Delta(\mathbf{k})$ is. It requires some sort of order, fluctuating or otherwise, or a new bosonic degree of freedom. While YRZ proposed Eq. (1.1) phenomenologically, their intuition was based on weak-coupling RPA diagrammatics³¹ on two-leg ladder systems. In the context of an algebraic charge liquid,³² Qi and Sachdev²⁹ also obtained Eq. (1.1). Thus far, the only system shown to have the properties of an algebraic charge liquid is one with parameters radically different from those of the cuprates.³³

Our point here is that $\Delta(\mathbf{k})$ arises fundamentally from a new degree of freedom associated with dynamical spectral weight transfer. Ideally, it would be advantageous to derive Eq. (1.1) directly from the strong-coupling parameter space of the basic model for a doped Mott insulator, for example, the Hubbard model. Such a derivation has not been presented in the literature. Hence, it is this problem that we address. Since zeros^{24,25} arise from a cancellation of the spectral weight in the

upper and lower Hubbard bands (hereafter UHBs and LHBs), an accurate description of the upper band is required in a derivation of Eq. (1.1). Hence, an attempt to obtain Eq. (1.1) from a model that projects out the UHB, for example, the $t - J$ model, is initially a nonstarter, as this model does not have zeros of the type required for Eq. (1.1). Nonetheless, the information regarding the UHB should be correctly encoded into a theory of the lower band if the UHB is integrated out (rather than projected out) exactly *à la* Wilson.³⁴ In this paper, we show how the method we have recently developed^{35–37} for carrying out the Wilsonian program for the Hubbard model can be used to derive Eq. (1.1). We show explicitly that two types of excitations emerge, projected electrons (yielding poles in the propagator) and a new bound state that gives rise to zeros. The bound state is not made out of the elemental excitations and hence is orthogonal to an electron (hence the zero). It represents a charge e excitation that originates from the nonrigidity of the Hubbard bands, in other words, the well-documented dynamical spectral weight transfer,^{38–40} the key fingerprint of the breakdown of the band concept in Mott systems. Since the mathematics of Fermi arcs requires two kinds of excitations, one with poles and the other with zeros, we refer to a physical model that contains both, such as the one presented here, as the standard model. More exotic models relying on some type of order would fall outside this framework.

II. CHARGE $2e$ BOSON THEORY

A. Preliminaries

Underlying our toy Green function is a two-pole structure of the form

$$G_{\text{toy}}(\omega, \mathbf{k}) = Z \left(\frac{\cos^2 \theta}{\omega - \omega_+} + \frac{\sin^2 \theta}{\omega - \omega_-} \right). \quad (2.1)$$

Here $\cos^2 \theta = (\omega_+ - \varepsilon(\mathbf{k})) / (\omega_- - \omega_+)$ and $\omega_{\pm} = \frac{1}{2}(\varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k}) \pm \sqrt{(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}))^2 + 4|\Delta(\mathbf{k})|^2})$. Zeros arise from the interference between the poles at ω_- and ω_+ . Any model that admits zeros must have at least this two-pole structure. There are two limits of the Hubbard model in which the zero surface can be calculated exactly. In the atomic limit, the zero surface of the exact single-particle Green function,

$$G^R(\omega) = \frac{1+x}{\omega - \mu + \frac{U}{2}} + \frac{1-x}{\omega - \mu - \frac{U}{2}}, \quad (2.2)$$

is independent of the momentum given by $\omega = \mu$ and $x = 0$. When the hopping is nonzero, $t \neq 0$, the only limit in which the zero surface can be calculated exactly is at half-filling and particle-hole symmetry. In this limit, the zero surface²⁴ for a nearest-neighbor band structure is the magnetic Brillouin zone. Since Fermi arcs are absent from both the atomic limit and the half-filled system with hopping, it follows necessarily that Fermi arcs (if they are present at all in the Hubbard model) arise entirely from the dynamical part of the spectral weight.

Dynamical spectral weight transfer represents a concrete example of more being totally different. As is evident from Eq. (2.2), the weight of the lower band in the atomic limit is $1+x$. This spectral weight has a natural interpretation in terms of electron states. There are $2x$ electron addition and $1-x$

electron removal states. Hence, in the atomic limit, there is a one-to-one correspondence with the spectral intensity and the number of electron states in the lower band. When the hopping is turned on, the spectral intensity increases in the lower band to $1+x+\alpha$, where

$$\alpha = \frac{2t}{U} \frac{1}{N} \sum_{ij,\sigma} \langle f_{i\sigma}^\dagger f_{j\sigma} \rangle + O((t/U)^2) \quad (2.3)$$

and the $f_{i\sigma}$'s are a rotation of the original fermionic operators in the Hubbard model such that it is block diagonal. The energy of each block is nU , with n the number of double occupancies in each block. α is necessarily positive because any hopping process that creates double occupancy decreases the available spectral weight in the upper band. Consequently, counting electrons, fractionalized or otherwise, cannot exhaust the total number of degrees of freedom in the lower band. A new degree of freedom must be present which is distinct and hence orthogonal to electron quasiparticles. This degree of freedom will appear as a 0 in the spectral function in the lower band. It is precisely the nature of the states that arise from the mixing with the upper band that we elucidate here.

Several approaches suggest some kind of composite excitation mediates Fermi arcs. Consider the $SU(2)$ gauge theory of the $t-J$ model proposed by Wen and Lee⁴¹ in which the elemental fields are the appropriate linear combinations of two charge e bosons and two spinons. A mean-field calculation⁴¹ of the coherent spinon-boson Green function reveals that the spectral weight of the occupied part of the spectrum exceeds $1-x$, acquiring a value of $1+x/2$ instead. Wen and Lee⁴¹ alleviated this problem by introducing an interaction which recombined the bosons and fermions back into the elemental fields. The effect of this interaction with strength U was to enhance the spectral weight in the unoccupied part of the spectrum. The correct spectral weights were obtained simply by adjusting the magnitude of U . The unoccupied part of the spectrum⁴¹ shows up as a small hole pocket centered roughly at $(\pi/2, \pi/2)$. The intensity on the back-side of the pocket is greatly suppressed, thereby leading to a structure not too distinct from a Fermi arc. Subsequent work on the $U(1)$ formulation of the $t-J$ model with a phenomenological spinon-holon binding term reached a similar conclusion.⁴² However, the most extensive calculation in the gauge theoretic formulations of the Hubbard model reached a rather different conclusion. Working directly with the Hubbard model, Imada and colleagues¹⁹ used a slave-particle construction with the gauge fluctuations treated at the RPA level and concluded it is actually dynamical spectral weight transfer that leads to a fermi arc structure and a Green function of the YRZ form. Aside from suffering from the lack of a systematic way of treating the gauge fluctuations, this formulation generates Fermi arcs from a neutral composite excitation.¹⁹ Since neutral entities cannot couple to the current, it is unclear how such entities can influence the spectral function. What we demonstrate here is that dynamical spectral weight transfer mediates Fermi arcs.

B. Exact results: The conserved charge and the low-energy mode

Dynamical spectral weight transfer has two profound consequences. First, we show exactly that the conserved

charge $(1 - x)$ is not exhausted by counting the degrees of freedom minimally coupled to the electromagnetic gauge. The remainder are carried by an incoherent background. Second, the dynamically transferred degrees of freedom give rise to zeros in the lower band. In fact, the physics we find here is analogous to the finite U charge processes that contribute to the spectral function measured by ARPES in heavy fermions.⁴³

We start with the procedure to integrate out the UHB. Previously, we demonstrated^{35–37} that a theory of the LHB (hole doping) can be obtained by introducing a new fermionic field D_i ^{35,36} which represents the excitations in the upper band. This field has mass U and hence should be integrated out to construct the exact low-energy theory. As in the derivation of all collective phenomena which dates back to the classic paper of Bohm and Pines,⁴⁴ a constraint must be introduced so that, when solved, the model in the extended space is equivalent to the starting UV-complete theory. The new fermionic degree of freedom enters the action in a quadratic fashion and hence the standard fermionic path integral techniques can be applied to integrate the high-energy scale of the UHB. Since the LHB and UHB are not rigid in the sense that the spectral weights of the two bands are coupled, integrating out the upper band will lead to new degrees of freedom in the lower band. In Euclidean signature, the Hubbard action in the extended space is

$$\begin{aligned} S_h^{\text{UV}} = \int_0^\beta d\tau \int d^2\theta \left\{ \bar{\theta} \theta \sum_{i,\sigma} (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* \partial_\tau c_{i\sigma} \right. \\ + \sum_i D_i^* \partial_\tau D_i + U \sum_j D_j^* D_j - t \sum_{i,j,\sigma} g_{ij} [\bar{\theta} \theta (1 - n_{i\bar{\sigma}}) \\ \times (1 - n_{j\bar{\sigma}}) c_{i\sigma}^* c_{j\sigma} + D_i^* c_{j\sigma}^* c_{i\sigma} D_j + (D_j^* \theta c_{i\sigma} V_\sigma c_{j\bar{\sigma}} \\ \left. + \text{C.c.}) \right] + s \bar{\theta} \sum_j \varphi_j^* (D_j - \theta c_{j\uparrow} c_{j\downarrow}) + \text{C.c.} \left. \right\}, \quad (2.4) \end{aligned}$$

where the matrix g_{ij} selects the relevant neighbors, $V_\sigma = \pm 1$ ($\sigma = \uparrow, \downarrow$), the constraint is given by $\delta(D_i - \theta c_{i\uparrow} c_{i\downarrow})$, θ is a Grassmann, s is a constant with units of energy so that φ_i is dimensionless, and $c_{i\sigma}$ is an electron annihilation operator for site i with spin σ . Because the δ -function constraint appears exponentiated in the action, an auxiliary field with charge $2e$, φ_i , enters the action as a Lagrange multiplier. As a consequence, the field φ is not made out of the elemental excitations (thereby distinguishing it from other charge $2e$ scenarios involving pairs of electrons) but, rather, arises because the UHB and LHB are not rigid bands. In the action, the first two terms represent the dynamics in the LHB and UHB, respectively; the third term, the mass of the D field; the fourth term, the hopping in the lower band with matrix element t ; the next two, the dynamical mixing between the upper and lower bands; and the last term, the constraint. The constant s has units of energy and is $O(t)$.⁴⁵ It is straightforward to check that solving the constraint by integrating out the auxiliary field, φ_i , followed by an integration over D_i exactly reduces S_h^{UV} to the action for the standard Hubbard model. This is the UV limit of our theory. The advantage of the reformulation above is that it cleanly associates the physics of the upper band with a fermionic field D_i which enters the action in a quadratic fashion. To obtain the IR limit, one simply has to perform the Gaussian integration over the massive field, D_i .

The result is the low-energy or IR action, $S_h^{\text{IR}} = \int d\tau \mathcal{L}_h^{\text{IR}}$, with the associated Lagrangian,

$$\begin{aligned} \mathcal{L}_h^{\text{IR}} = (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* \partial_\tau c_{i\sigma} - t g_{ij} (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* c_{j\sigma} (1 - n_{j\bar{\sigma}}) \\ - (s\varphi_i - tb_i)^* (\mathcal{M}^{-1})_{ij} (s\varphi_j - tb_j) \\ - (s\varphi_i^* c_{i\uparrow} c_{i\downarrow} + \text{c.c.}) - \frac{1}{\beta} \text{tr} \ln \mathcal{M}, \quad (2.5) \end{aligned}$$

where a matrix element of \mathcal{M} is given by $\mathcal{M}_{ij} = (\partial_\tau + U)\delta_{ij} - t g_{ij} c_{j\sigma}^\dagger c_{i\sigma}$ and $b_i = \sum_j g_{ij} c_{j\sigma} V_\sigma c_{i\bar{\sigma}}$. Hereafter, repeated indices are implicitly summed unless otherwise stated. It is important to note that no approximations have been made as of yet.

In both actions, S_h^{UV} and S_h^{IR} , global U(1) symmetry guarantees the existence of a conserved charge, which turns out to be

$$\begin{aligned} Q_h^{\text{UV}} = (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* c_{i\sigma} + 2D_i^* D_i, \quad (2.6) \\ Q_h^{\text{IR}} = (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* c_{i\sigma} + 2(s\varphi_i - tb_i)^* \\ \times (\mathcal{M}^{-1})_{ik} (\mathcal{M}^{-1})_{kj} (s\varphi_j - tb_j). \quad (2.7) \end{aligned}$$

It is a natural consequence that the conserved charge $\langle Q_h^{\text{UV}} \rangle$ is consistent with the number of electrons in the original Hubbard model since the operator $D_i^\dagger D_i$ counts the number of doubly occupied sites. From the Hellman-Feynmann theorem, it is straightforward to check how the number of double occupancies, $n_{\text{docc}}^{\text{UV/IR}}$, is related to D_i . Since $n_{\text{docc}}^{\text{UV/IR}} = \beta^{-1} \partial \ln \mathcal{Z}_h^{\text{UV/IR}} / \partial U$ with $\mathcal{Z}_h = \int D[\dots] e^{-S_h}$, one can easily observe the second terms in Eqs. (2.6) and (2.7) are identical to $n_{\text{docc}}^{\text{UV}}$ and $n_{\text{docc}}^{\text{IR}}$, respectively. As a result, the conserved charge $\langle Q_h^{\text{IR}} \rangle$ is identified with the number of electrons, $1 - x$, with x the number of holes. This is one of the indications that the low-energy action, S_h^{IR} , retains the structure of the Hubbard model even after the integration of the massive modes.

Another advantage of the low-energy theory is that the non-Fermi-liquid nature of the low-energy excitations is immediately manifest. To illustrate this, one can add a minimally coupled source term,³⁶

$$\mathcal{L}_h^{\text{UV}} = J_{i\sigma}^* [\bar{\theta} \theta (1 - n_{i\bar{\sigma}}) c_{i\sigma} + \bar{\theta} c_{i\bar{\sigma}}^* V_\sigma D_i] + \text{c.c.}, \quad (2.8)$$

so that when the constraint is solved, the bare electron operator is generated.³⁶ What we would like to know is what is the transformed fermion at low energies. Integrating out the D_i fields results in a source contribution to the IR Lagrangian,

$$\mathcal{L}_h^{\text{IR}} = J_{i\sigma}^* \psi_{i\sigma} + \text{c.c.} - J_{i\sigma}^* c_{i\bar{\sigma}}^* (\mathcal{M}^{-1})_{ij} c_{j\bar{\sigma}} J_{j\sigma}, \quad (2.9)$$

with a new collective field, $\psi_{i\sigma}$, given by

$$\psi_{i\sigma}^* = (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* + t b_j^* (\mathcal{M}^{-1})_{ji} V_\sigma c_{i\bar{\sigma}} - s \varphi_j^* (\mathcal{M}^{-1})_{ji} V_\sigma c_{i\bar{\sigma}}. \quad (2.10)$$

Note $\psi_{i\sigma}$ is derived not contrived. It is Eq. (9) in Ref. 35. We obtained it by integrating the UV-complete Lagrangian in the presence of the source term that generates the correct UV current with respect to the massive field D_i . $\psi_{i\sigma}$ is the propagating degree of freedom in the IR. It contains not only an electron-like quasiparticle affected by nearby spin fluctuations, but also a hole (with the opposite spin) that is dressed with a doubly charged bosonic mode. Note that we cannot give $\psi_{i\sigma}$ a simple interpretation in terms of bosons or fermions. At best,

$\psi_{i\sigma}$ corresponds to the physical field that is minimally coupled to an external gauge field. That is, these are the excitations that couple to light. Hence, it is the field that is probed by an ARPES experiment, for example. While $\psi_{i\sigma}$ was derived earlier, what we did not show explicitly is that it does not stand in a one-to-one correspondence with the bare electrons. This can be proven exactly by focusing on the positive-definite quantity,

$$\begin{aligned} \psi_{i\sigma}^* \psi_{i\sigma} &= (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* c_{i\sigma} + (tb - s\varphi)_j^* (\mathcal{M}^{-1})_{ji} c_{i\bar{\sigma}} c_{i\bar{\sigma}}^* \\ &\quad \times (\mathcal{M}^{-1})_{ij} (tb - s\varphi)_j \\ &= Q_h^{\text{IR}} - (tb - s\varphi)_j^* (\mathcal{M}^{-1})_{ji} (2 + c_{i\bar{\sigma}}^* c_{i\bar{\sigma}}) (\mathcal{M}^{-1})_{ij} \\ &\quad \times (tb - s\varphi)_j, \end{aligned} \quad (2.11)$$

which is essentially the conserved charge less the number of doubly occupied sites. Since the second term in the last line is positive definite, the number of low-energy collective modes which are minimally coupled to the electromagnetic gauge field is less than $\langle Q_h^{\text{IR}} \rangle = 1 - x$. The natural resolution of this conundrum is that the number operator only counts those excitations that have a particle-like interpretation. That is, the number operator only counts the coherent part of the spectrum. All of the stuff mediated by mixing with the upper band is entirely incoherent, and hence while it can contribute to the current, it is not enumerated by counting the number of particles. The remainder of the charge count is carried by the last term in Eq. (2.9).

This discrepancy is not a surprise when one considers that the total spectral weight of the lower band exceeds $1 + x$ (Refs. 38 and 40) by a dynamical correction, $\alpha > 0$, that depends on the hopping integral, t . Since there are only $1 + x$ electron states in the lower band, and only charge e excitations contribute to the spectral function, there has to be some new charge mode to make up the difference. What $\psi_{i\sigma}$ makes plain is that there are charge e states that contribute to the current that are completely incoherent. It is a composite excitation of φ^\dagger and a hole $c_{i\bar{\sigma}}$. In terms of the UV variables, this degree of freedom represents the binding of a doublon and a holon. The new composite excitation, $\varphi^* \mathcal{M}^{-1} V_\sigma c_{i\bar{\sigma}}$, has internal structure and hence is orthogonal to the projected electron. Since there is no Hilbert space for φ , interpreting $\varphi^\dagger c_{i\bar{\sigma}}$ in terms of a particle is not possible. It is this additional degree of freedom that creates the Fermi arc structure—that is, the zeros of the Green function. Hence, hidden in $\psi_{i\sigma}$ is an incoherent contribution to the single-particle Green function. What this discussion makes clear is that φ should not be considered to be an independent degree of freedom but, rather, one that is strongly coupled to the fermions.

What we have shown thus far is that there is a dynamical contribution to the charge degrees of freedom that are coupled to the source term that generates the current. Such entities are the physical degrees of freedom that create holes in the lower band. Consequently, when one such excitation is removed from the lower band, the change in the spectral weight should also depend on t . Hence, the doping level should receive a dynamical contribution. To this end, we defined⁴⁶ $x' = x + \alpha$, and hence the weight in the UHB is $1 - x'$ and the occupied and empty parts of the lower band are $1 - x'$ and $2x'$, respectively.

C. Green function and approximations

Thus far, all of our statements are exact. Our calculation of the Green function is not, however. To lend credence to our treatment, we state our assumptions clearly and up front. The complexity arises in treating the φ degree of freedom. Our treatment is in the spirit of the results obtained in the previous section, namely, that φ leads to the creation of a new charge e excitation that is orthogonal to a projected electron on account of its internal structure.

Having determined the generating functional, $\mathcal{L}_h[\{J_{i\sigma}^*, J_{i\sigma}\}]$, we proceed to calculate the Green function. In the functional formalism, it is given by

$$\begin{aligned} G_\psi(\mathbf{r}_i - \mathbf{r}_j, \tau) &= -\frac{\delta^2}{\delta J_{i\sigma} \delta J_{j\sigma}^*} \ln \mathcal{Z}_h^{\text{IR}}[\{J_{i\sigma}^*, J_{i\sigma}\}]|_{J^*=J=0} \\ &= -\langle \mathcal{T}_\tau \psi_i(\tau) \psi_j^\dagger(0) \rangle + \langle \delta(\tau) c_{i\bar{\sigma}}^\dagger (\mathcal{M}^{-1})_{ij} c_{j\bar{\sigma}} \rangle, \end{aligned} \quad (2.12)$$

where \mathcal{T}_τ represents time ordering and $\langle \dots \rangle$ stands for the average over all possible paths. Since the second term is independent of time, this term contributes to the incoherent part of the Green function. To understand the first term which contains both coherent and incoherent responses, it is sufficient to focus on the correlator between the $\psi_{i\sigma}$'s. Since $\psi_{i\sigma}$ contains a composite excitation which has a prefactor of t/U , $\langle \mathcal{T}_\tau \psi_{i\sigma}(\tau) \psi_{j\sigma}^\dagger(0) \rangle$ can, in principle, be expanded in power of t/U . The presence of the projection operator, $(1 - n_{i\bar{\sigma}})$, however, does not necessarily guarantee that it gives a dominant contribution compared to the composite entities.

For the purpose of numerical evaluation, we make an approximation to the projection operators, following the idea developed by Zhang *et al.*⁴⁷ However, the crucial difference is that we make the substitution the bare hole concentration by the effective hole doping level ($x \rightarrow x'$), since the physical entities coupled to the external gauge field are not the bare electrons but are, rather, dynamically generated. Hence our first approximation is

$$(A1) \quad (1 - n_{i\bar{\sigma}}) c_{i\sigma}^* c_{j\sigma} (1 - n_{j\bar{\sigma}}) \rightarrow g_t c_{i\sigma}^* c_{j\sigma},$$

where $g_t = 2x'/(1 + x')$. Interestingly, in the strong coupling limit, ($U/t \gg 1$), a mean-field approach to Kotliar-Ruckenstein's slave boson construction⁴⁸ led to the same renormalization factor for the charged fermion but with x' replaced with x . Likewise,

$$(A2) \quad (1 - n_{i\bar{\sigma}}) c_{i\sigma}^\dagger (\partial_\tau + \dots) c_{i\sigma} \rightarrow g_p c_{i\sigma}^\dagger (\partial_\tau + \dots) c_{i\sigma},$$

where $g_p = (1 - x')/(1 - x)$. The multiplicative factors are chosen here for internal consistency with the two assumptions.

Since the action $\mathcal{S}_h^{\text{IR}}$ has all relevant degrees of freedom for the low-energy sector, including the spin singlet fluctuations (b_i) and mixing between the separate Hubbard bands (φ), it is reasonable to expand the action in powers of t/U . To leading order, the matrix elements $(\mathcal{M}^{-1})_{ij}$ is $U^{-1} \delta_{ij}$. From the fact that the collective boson φ_i only has dynamics through its coupling to the fermions, we assume the dynamics of the boson to be frozen. Operationally this assumption breaks down at $O(t/U)^2$, where the explicit dynamics of φ appears, as can be seen from an expansion of the \mathcal{M} matrix, $\frac{s^2}{U^2} \varphi^* (\partial_\tau - U + \dots) \varphi$.

In fact, even at $O(t/U)^2$, the propagator for φ makes plain that it has a pole only in the high-energy sector. This justifies the assumption that

(A3) the bosonic field, φ , has no dynamics in the LHB.

In other words, it alone is highly massive and is not likely to propagate in the low-energy sector. Finally, although local spin ordering might be non-negligible, we assume it to be, at most, ancillary to the strong interaction physics arising from the coupled boson-fermion terms. This is a key assumption and certainly not traditional, as most treatments of the LHB focus on the spin physics. However, as our emphasis here is on isolating the source of zeros in the LHB, demonstrating that the action possesses such modes in the absence of the spin-spin scattering term would suffice to show that such an interaction is indeed ancillary to the essential charge physics. As will become evident, our treatment does in fact show this to be the case. Under these considerations, the effective low-energy action turns into

$$\begin{aligned} \mathcal{S}_h^{\text{IR}} = \int_0^\beta d\tau \left\{ c_{\mathbf{k}\sigma}^* [g_p(\partial_\tau - \mu)\delta_{ij} - g_t\epsilon_{\mathbf{k}}] c_{\mathbf{k}\sigma} \right. \\ \left. - \frac{1}{U^2} (s\varphi - tb)_q^* (U + 2\mu)(s\varphi - tb)_q \right. \\ \left. - (s\varphi_q^* c_{\mathbf{q}-\mathbf{k}\uparrow} c_{\mathbf{k}\downarrow} + \text{c.c.}) \right\}, \end{aligned} \quad (2.13)$$

where μ denotes the chemical potential, \mathbf{k} and \mathbf{q} are the momenta, and $\epsilon_{\mathbf{k}} = tg_{ij}e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)}$. This action has a BCS-like coupling and hence will have a Green function of the form of Eq. (1.1). That the Green function must be of the form of Eq. (1.1) is not dependent on the assumptions delineated earlier. It relies solely on the fact that the spectral weight in the lower band exceeds $1 + x$ and hence a new charge e state distinct from the projected electrons must be present. Such an excitation can only be a composite.

Consequently, for a given amplitude of $\varphi_{\mathbf{q}}$, the Fourier transformation of the two-point correlator $\mathcal{G} = -\langle \mathcal{T}_\tau \psi_i(\tau) \psi_j^\dagger(0) \rangle$ becomes

$$\mathcal{G}(i\omega_n, \mathbf{k}) = \frac{\tilde{g}_t}{i\omega_n - \mu - \tilde{g}_t\epsilon_{\mathbf{k}} - \Sigma_\pm(i\omega_n, \mathbf{k})} + \frac{t}{U}(\dots), \quad (2.14a)$$

$$\Sigma_\pm(i\omega_n, \mathbf{k}) = \frac{s_{\mathbf{k},\mathbf{q}}^2 \varphi_{\mathbf{q}} \varphi_{\mathbf{q}}^*}{i\omega_n - \mu \pm \tilde{g}_t\epsilon_{\mathbf{q}-\mathbf{k}}}, \quad (2.14b)$$

where $\omega_n = (2n + 1)\pi/\beta$ for $n \in \mathbb{Z}$, $\tilde{g}_t = g_t/g_p$, and $s_{\mathbf{k},\mathbf{q}} = 1 - (\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{q}-\mathbf{k}})/U$. The \pm subscript on the self-energy arises from the two choices which are possible for treating the dynamics of the charge $2e$ boson. If φ_i is treated as an independent degree of freedom that can condense, then it can be absorbed as a redefinition of the interaction strength, $s \rightarrow s\varphi$. This will correspond to a simple condensation of φ in a nonzero momentum particle-particle channel, hence the plus sign in front of the $\tilde{g}_t\epsilon_{\mathbf{q}-\mathbf{k}}$ factor in the denominator of the self-energy. As will be clear, this is not the interpretation of φ that is ultimately consistent with the theory outlined here. Alternatively, $\varphi_i^* c_{i\bar{\sigma}}$ could be viewed as a new composite charge e excitation that results from dynamical spectral weight transfer. With such bound modes, the interaction term, $\varphi^* c_\uparrow c_\downarrow$, can be interpreted

as a particle-hole scattering process. To implement this interpretation in the Green function, we note that since $\varphi^* c_\uparrow c_\downarrow$ now describes the scattering of an electron c_σ off a composite particle $\varphi^* V_\sigma c_{\bar{\sigma}}/|\varphi|$, the denominator in the one-loop self energy will resemble that of a particle-hole scattering event, thereby leading to a minus sign in front of the $\tilde{g}_t\epsilon_{\mathbf{q}-\mathbf{k}}$ term in the denominator of the self-energy. In addition, the ellipse in Eq. (2.14a) represents the terms that originate from the mixing between the composite excitations and the projected electron, which are at least suppressed by the factor t/U . The number \tilde{g}_t results from the rescaling $g_p^{1/2} c_{i\sigma} \rightarrow c_{i\sigma}$. Since $\tilde{g}_t = g_t/g_p \simeq 2x'$, the t/U corrections in Eq. (2.14a) are comparable to the leading term only for $x' < t/2U \sim 0.05$. For example, at half-filling, the Green function only has the t/U term and the spectral weight is governed entirely by the mixing between the projected and the composite excitations as shown previously.⁴⁵ In the current treatment, we explore entirely the contribution from the leading term, which is of the form of Eq. (1.1).

D. Free-energy minimum approach to the $2e$ boson

Evaluating the Green function is equivalent to a random-matrix problem. In the most general case, the field φ_i must be integrated over with a separate value on each site. However, such a multi-variable integration is not tractable in any dimension. From the observation that the collective boson is not canonical, that is, it does not have its own kinetics, it was previously conjectured that the spatially homogeneous configuration was the most prominent candidate for the ground state.^{35,45} Even though such an approach was successful in capturing some experimental⁴⁵ findings, it still leaves an open question whether the homogeneous solution minimizes the free energy. To this end, we explore some inhomogeneous solutions for φ_i to see where the free-energy is a minimum. In particular, we explore a staggered configuration, $\varphi_i = e^{i\mathbf{q}\cdot\mathbf{r}_i} |\varphi_0|$. It should be noted that a particular choice of the configuration of φ does not correspond to spontaneous symmetry breaking, since the bosonic mode is in lack of inherent dynamics.

In Fig. 1, we directly compute the free energy difference between a configuration with a spatial texture and the homogeneous state, $\Delta F = F(\varphi_0 e^{i\mathbf{q}\cdot\mathbf{r}}) - F(\varphi_0)$, where \mathbf{q} , determines the spatial dependence of φ_i . Except for small values of φ_0 in which the homogeneous solution minimizes the free energy, the distinct minimum occurs at (π, π) when the magnitude of the bosonic field, φ_0 , approaches unity. This is significant because the probability distribution of φ_0 computed from $P(|\varphi|) = 1/\mathcal{Z}_h^{\text{IR}} \int D[\{c, c^*\}] e^{-S_h^{\text{IR}}}$, has a distinct maximum precisely at the value of φ where the (π, π) solution minimizes the free energy. This state of affairs obtains because a quick inspection of the action reveals that for a staggered configuration of φ , the $\varphi^\dagger b$ term actually vanishes. This results in a lowering of the energy relative to the homogeneous solution.

That the (π, π) configuration of φ_i minimizes the free energy is highly significant because the evaluation any integral over φ_i will be dominated by the staggered solution. What about the single-particle Green function? In our previous treatment of this problem in which we assumed that the mixing with the UHB was mediated by a homogeneous boson, φ_0 for all sites, we obtained a completely gapped structure at

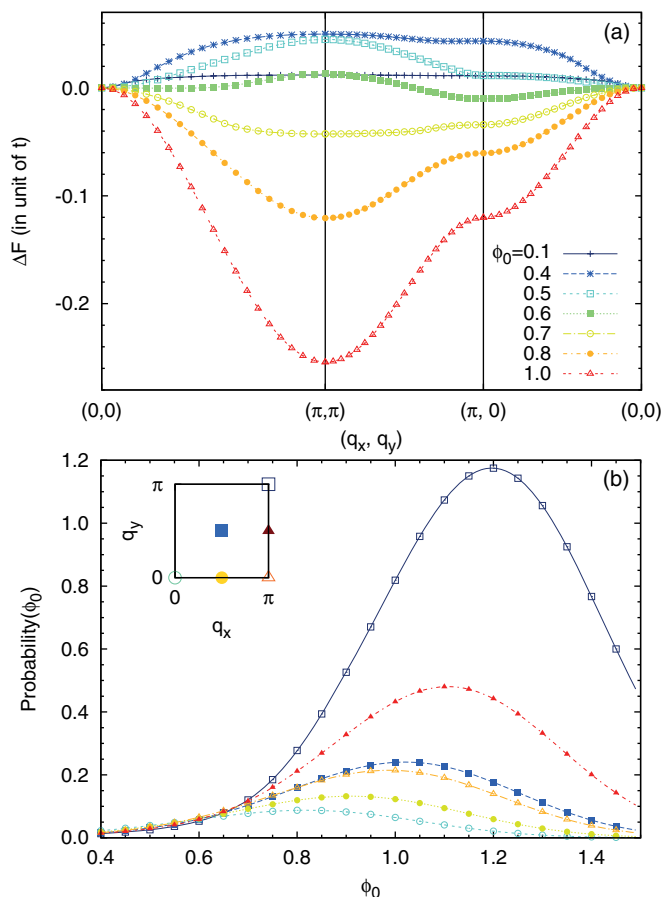


FIG. 1. (Color online) Free energy minimization and probability distribution of charge $2e$ boson. (a) $\Delta F = F(\varphi_0 e^{i\mathbf{q}\cdot\mathbf{r}}) - F(\varphi_0)$ as a function of momentum \mathbf{q} . φ_0 is the magnitude of the charge $2e$ boson. As is evident, the free energy is strongly dependent on the momentum. As φ_0 increases, the minimum of the free energy shifts to (π, π) . This corresponds to a sign change for the bosonic excitation around a plaquette. (b) Probability distribution for φ_0 evaluated from the IR action by the relation, $P(|\varphi|) = 1/\mathcal{Z}_h^{\text{IR}} \int D[\{c, c^*\}] e^{-S_h^{\text{IR}}}$. The maximum occurs at $\varphi_0 \approx 1.2$, where the corresponding momentum that minimizes the free energy is $\mathbf{q} = (\pi, \pi)$.

the chemical potential for the spectral function. Given that $\mathbf{q} = (\pi, \pi)$ is the global minimum, our expression for the Green function simplifies to

$$G(i\omega_n, \mathbf{k}) = \int d|\varphi| |\varphi| P(\varphi) \mathcal{G}(i\omega_n, \mathbf{k})|_{\varphi_q = \delta_{\mathbf{q}, \pi} |\varphi|}. \quad (2.15)$$

The probability distribution function $P(\varphi)$ is shown in Fig. 1(b). For completeness, we present in Fig. 2 the band dispersion corresponding to the maximum in the spectral function obtained from Eq. (2.14a) for three cases: (i) a homogeneous solution; (ii) a staggered (π, π) phase of φ_i in the particle-particle channel, Σ_+ ; and (iii) a staggered solution in the particle-hole channel, Σ_- . For the homogeneous phase, we find a hard gap [Fig. 2(a)] because no momentum states cross the chemical potential. However, as shown earlier, the homogeneous solution does not correspond to a minimum in the free energy. Consider the staggered solutions shown in Figs. 2(b) and 2(c). Figure 2(b) shows that even a staggered solution in the particle-particle channel, a gap does not occur

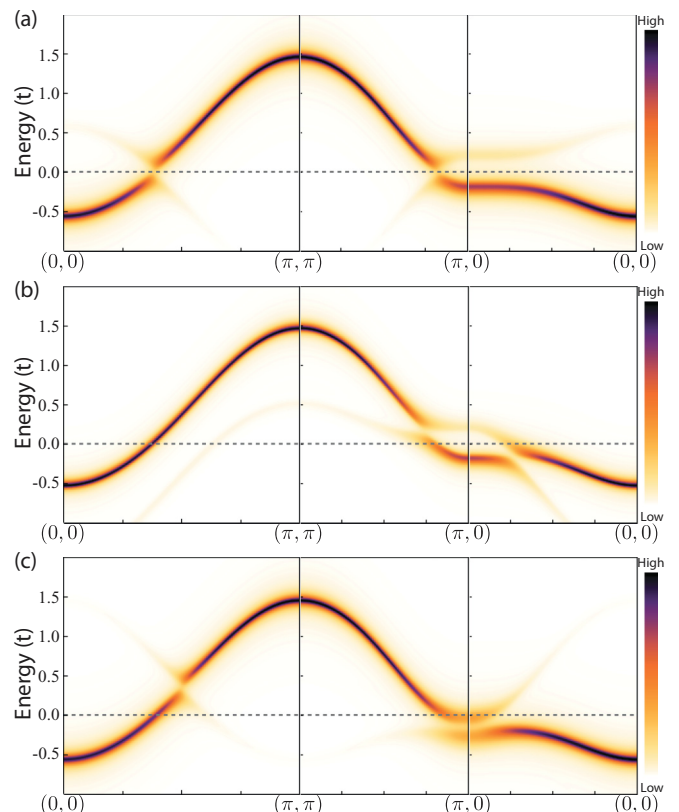


FIG. 2. (Color online) The low-energy band dispersion along high-symmetry directions for (a) a homogeneous configuration, $\varphi_i = \varphi_0$; (b) a staggered configuration ($\varphi_i = |\varphi_0| e^{i\pi \cdot r_i}$) evaluated by Eq. (2.14a); and (c) a staggered one evaluated by Eq. (2.14a). Here, we take the broadening factor $\eta = 0.025t$ for a typical value $U/t = 10$, $t'/t = -0.3$, $t''/t = 0.1$, and the bare hole doping level as $x = 0.12$. In the evaluation, the parameters, $\alpha = x' - x$ are taken from the numerical estimates of the number of double occupancies from Liebsch and Tong.⁴⁹

in the $(\pi, 0)$ region of the Brillouin zone. There is also a crossing along the zone diagonal. This indicates that a simple condensation of φ in a nonzero-momentum particle-particle channel cannot give rise to the nodal/antinodal dichotomy. There is in fact a clear reason why φ cannot be treated as an independent degree of freedom that can condense. There is a one-to-one correspondence between Eq. (2.10) and its analog [Eq. (19) in Ref. 39] in the standard perturbative treatment of the Hubbard model. In essence, the charge $2e$ boson replaces a string of operators that account for the mixing of double occupancy into the lower band. This is why this approach is simpler. As it would be completely incorrect to replace that string of operators with an average value, it is equally wrong to treat φ as a variable that can condense. In fact, it is well known⁴⁰ that such mean-field truncations fail to describe dynamical spectral weight transfer in the Hubbard model.

Consider the third dispersion [Fig. 2(c)], in which φ is the mediator of a composite charge e state. This corresponds to a self-energy given by Σ_- . The break in the dispersion just above the chemical potential is not followed by a re-entrant crossing at a higher momentum. Such a re-entrant crossing would give rise to a closed Fermi surface. It is the presence of

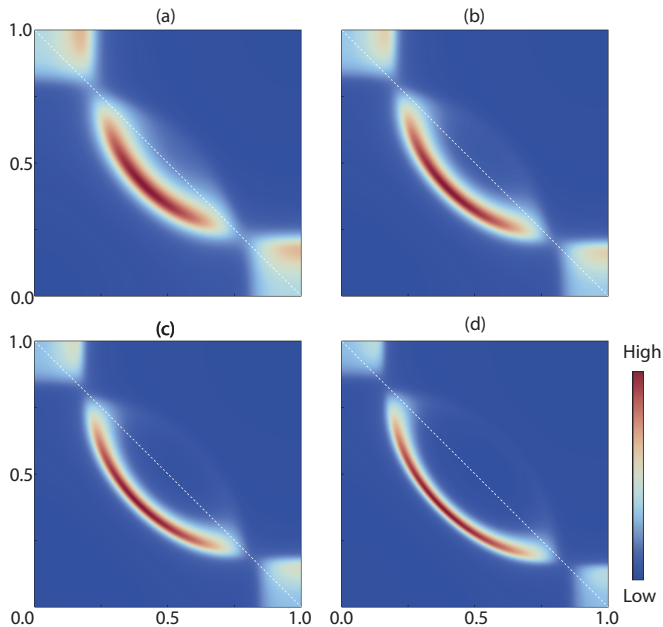


FIG. 3. (Color online) The spectral function of the low-energy theory for each hole doping level: (a) $x = 0.05$, (b) $x = 0.08$, (c) $x = 0.12$, and (d) $x = 0.18$. An incoherent background is removed and the intensities of the spectral function are normalized for the first quadrant of the full Brillouin zone.

the additional propagating degree of freedom which thwarts this re-entrance. In addition, there is no crossing at $(\pi, 0)$, but a broad incoherent feature indicative of the pseudogap. Since the breakup of the bound state results in a band crossing near the $(\pi, 0)$ region, the root cause of the pseudogap is the bound state formed between the bosonic field, φ , and a hole, as we have advocated previously.⁴⁵ Consequently, the pseudogap problem is one of confinement. The corresponding Fermi surfaces are shown in Fig. 3. The arc-like structure is evident. The line of zeros is given by the divergence of the self-energy and hence it is doublon-holon binding that is responsible for killing the intensity on the back side of the arc. The Fermi surfaces evolve smoothly for the doping levels shown from $x = 0.05$ to $x = 0.18$. Note also the broad feature at the zone boundary. While it is tempting to interpret the broad peak near the antinodal region as an electron pocket, the lack of coherent excitations makes this view untenable.

III. FINAL REMARKS

The key point this work demonstrates is that two types of charge carriers go into forming Fermi arcs. The projected

electrons are present in any low-energy reduction of the Hubbard model and create the spectral weight on the high-intensity side of the arc. The zeros correspond to composite excitations which are present as a result of dynamical spectral weight transfer and hence are present only if the UHB is retained or treated appropriately. Such composite excitations enter the self-energy through the particle-hole channel, as the relevant scattering process is that of a fermion from the composite excitation. Both of these features leading to an effective two-fluid model^{45,50} are present within a Wilsonian reduction of the high-energy scale in the Hubbard model. The treatment we have derived here should be valid as long as the UHB provides a relevant perturbation to the physics of the LHB. Hence, it cannot describe the crossover to the Fermi liquid regime in which φ is unbound. Experimentally, a decoupling of the UHB from the LHB appears to take place around $x \approx 0.25$.⁵¹ Accompanying the collapse is a transition from a small Fermi surface scaling with x to a large one with effective area $1 - x$. The precise nature of this transition will be the subject of a future study. However, a prediction of this work is that in the pseudogap regime, the volume of the Fermi arc region should be given by x' rather than x . This follows from the fact that the number of particle-like excitations that minimally couple to the electromagnetic gauge is less than $1 - x' < 1 - x$. Hence, the hole Fermi surface should be given by x' . High-precision ARPES measurements can be employed to verify this result.

Since our scheme of two types of charge carriers, one giving rise to zeros and the other to poles, seems quite general, it is tempting to rewrite the IR theory in terms of the composite and projected excitations. This would require integrating in an additional field for the composite, $f_{i\sigma}$, degree of freedom. The composite fermion is not canonical, however, and treating it as such would destroy the key feature leading to a suppression of the spectral on the back side of the arc. Thus far, we have found no consistent way of doing this. Hence, an open problem remains precisely how the new composite excitation should be treated. But that it is present in any standard model of Fermi arcs is not in doubt.

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