The Mott transition as a topological phase transition

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We show that the Mott metal-insulator transition in the standard one-band Hubbard model can be understood as a topological phase transition. Our approach is inspired by the observation that the mid-gap pole in the self-energy of a Mott insulator resembles the zero-energy spectral pole of the localized surface state in a topological insulator. We use NRG-DMFT to solve the infinite-dimensional Hubbard model, and represent the resulting local self-energy in terms of the boundary Green’s function of an auxiliary tight-binding chain without interactions. The auxiliary system is of generalized SSH model type; the Mott transition corresponds to a dissociation of domain walls.

Recently, the violation of Luttinger’s theorem in correlated materials has been connected to the emergence of topological order [34–42]. Although Luttinger’s theorem is satisfied throughout the FL phase of the Hubbard model due to the vanishing of the Luttinger integral [9, 42–45], it is violated in a MI [9, 43, 46]. Importantly, the Luttinger integral takes a universal finite value throughout the MI phase [9], suggesting that it may play the role of a topological invariant, and that topological information is contained in the interaction self-energy.

In this Letter, we uncover a hidden topology in the self-energy of the standard one-band paramagnetic Hubbard model in infinite dimensions. Specifically, we show that the rich many-body features of the Mott transition can be interpreted in terms of topological properties of an auxiliary non-interacting system coupled to the physical lattice degrees of freedom. The original interacting lattice system is mapped onto a completely non-interacting one; the self-energy dynamics are provided by coupling to fictitious degrees of freedom of an auxiliary system, see Fig. 1. We use NRG-DMFT [6, 7, 47] to calculate the zero-temperature local lattice self-energy numerically exactly, perform the exact mapping to an auxiliary tight-binding chain coupled to each physical lattice site, and analyze their topological properties across the Mott transition. The auxiliary chains are found to be of generalized Su-Schreiffer-Heeger [48] (SSH) model type, with the MI being the topologically nontrivial phase. The double peak structure of the self-energy in the topologically trivial FL phase corresponds to an SSH chain with additional domain walls. In each regime, we construct simple effective models to describe the emergent physics.

Figure 1. Mapping from the Hubbard model (left) to a fully non-interacting system (right) in which physical degrees of freedom (◦) couple to auxiliary tight-binding chains (□).

The Mott transition is a classic paradigm in the physics of strongly correlated electron systems, where electronic interactions drive a metal-insulator phase transition [1–3]. In a Mott insulator (MI), the strong local Coulomb repulsion localizes electrons, opening a charge gap to single-particle excitations and suppressing transport.

Although most MIs are accompanied by magnetic order at low temperatures, yielding a symmetry-broken superlattice structure [2], this is not an essential requirement [3–5]. The one-band Hubbard model on the Bethe lattice is the simplest model describing the Mott transition to a paramagnetic MI, and can be solved numerically exactly using dynamical mean-field theory (DMFT) [6, 7]. The insulating properties of the MI cannot be understood on the single-particle level; all nontrivial physics is contained in the interaction self-energy [7–9]. Throughout the insulating phase, the MI self-energy features a mid-gap pole pinned at zero energy. In the metallic Fermi liquid (FL) phase, Landau damping sets in at low energies. Close to the Mott transition, the FL self-energy develops a double-peak structure responsible for the pre-formed spectral gap, separating the central quasiparticle resonance in the density of states from the high energy Hubbard bands. Importantly, the Mott transition from FL to MI arises without the gap between the Hubbard bands closing; instead the self-energy peaks sharpen and coalesce to form a single Mott pole [7–9].

MIs contrast to standard band insulators, where the non-interacting band structure is already gapped due to the specific periodic structure of the real-space lattice. Indeed, the topology of the band structure of non-interacting systems plays an important role [10–12]. In particular, topological insulators constitute distinct phases of matter, characterized by robust metallic states localized at boundaries, or at interfaces with trivial insulators [13–15]. Topological phase transitions typically involve bulk gap closing without symmetry breaking, and are characterized by the discrete change in a topological invariant [16]. However, for interacting systems the standard topological classification breaks down [17–19]. The effect of including electronic interactions in systems with topologically nontrivial single-particle band structures is the focus of active research [20–33].
Models and mappings.—To uncover the topological features of the Mott transition in their simplest form, we focus on the one-band Hubbard model (Fig. 1, left),

\[ H_{\text{latt}} = H_{\text{band}} + H_{\text{int}} = \tilde{t} \sum_{\langle \langle i,j \rangle \rangle, \sigma} c_{\sigma}^\dagger c_{\sigma} + U \sum_i c_{i \sigma}^\dagger c_{i \sigma}^\dagger c_{i \sigma} c_{i \sigma}, \]

where \( \langle \langle i,j \rangle \rangle \) denotes nearest neighbours on the Bethe lattice, and we consider the system at half-filling for simplicity. In the limit of infinite lattice coordination \( N \to \infty \) (considered hereafter), the self-energy \( \Sigma(\omega) \) becomes purely local [6] such that \( G(\omega) = 1/(\omega^+ - \Sigma(\omega) - t^2 G(\omega)) \), where \( \omega^+ = \omega + i0^+ \), \( t = i\sqrt{N} \), and \( G(\omega) \) is the retarded lattice Green’s function.

Since the self-energy is analytic and causal, it may be replaced by a hybridization \( \Sigma(\omega) \equiv \Delta_0(\omega) \) to auxiliary (‘ghost’) degrees of freedom described by some non-interacting \( H_{\text{aux}} \). The full single-particle dynamics of Eq. 1 can therefore be reproduced by replacing \( H_{\text{int}} \to H_{\text{aux}} + H_{\text{hyb}} \). Specifically, we take \( H_{\text{aux}} \) to be non-interacting semi-infinite tight-binding chains,

\[ H_{\text{aux}} = \sum_{i, \sigma} \sum_{n=1}^{\infty} t_n \left( f_{i\sigma,n}^\dagger f_{i\sigma,n+1} + \text{H.c.} \right), \]

coupled at one end to the physical lattice degrees of freedom \( H_{\text{hyb}} = V \sum_{i, \sigma} \left( c_{i\sigma} f_{i\sigma,1} + f_{i\sigma,n}^\dagger c_{i\sigma} \right) \), see Fig. 1 (right). Here we use NRG-DMFT [7, 47] to determine \( \Sigma(\omega) \) at \( T = 0 \) for different \( U/t \) across the Mott transition, occurring at \( U_c/t \approx 5.9 \), and from it extract \( \{ t_n \} \).

Continued fraction expansion.—With \( H_{\text{aux}} \) in the form of a linear chain, \( \Delta_0(\omega) \) can be expressed as a continued fraction from the recursion \( \Delta_n(\omega) = t_n^2/\omega^+ - \Delta_{n+1}(\omega) \), where \( t_0 = V \). The set of chain hopping parameters \( \{ t_n \} \) in Eq. 2 for a given input self-energy \( \Sigma(\omega) \) is uniquely determined using this recursion for \( \Delta_n \) (initialized by \( \Delta_0 = \Sigma \)), together with the identity \( t_n^2 = -\frac{1}{2} \text{Im} \int d\omega \Delta_n(\omega) \). We impose a high-energy cutoff \( D \) such that \( \text{Im}\Sigma(\omega) \propto \theta(D - |\omega|) \) [49]. The mapping is efficient, numerically stable and accurate, although care must be taken with poles in \( \Delta_n \) [50].

Mott insulator.—For interaction strength \( U > U_c \), the Hubbard model Eq. 1 describes a MI, with two Hubbard bands separated by a hard spectral gap of width \( 2\delta \). The corresponding self-energy at zero temperature is shown in Fig. 2(a), obtained by NRG-DMFT for \( U/t = 9 \). The imaginary part of the self-energy features a mid-gap ‘Mott pole’ throughout the MI phase, pinned at \( \omega = 0 \) (and with finite weight at the transition).

Mapping to the auxiliary non-interacting chain, Eq. 2, leads to a model of modified SSH type — see Fig. 2(b). In particular, the hard gap in \( \text{Im}\Sigma(\omega) \) generates an alternating sequence of \( t_n \) in \( H_{\text{aux}} \) at large distances from the physical degrees of freedom,

\[ t_n \sim \frac{n^\delta}{D^{\delta + 1}} = \frac{1}{2} [D + (-1)^n \delta] : \text{MI} \]

In the MI phase, the auxiliary chain parameters are alternating for all \( n \), starting from a weak bond \( (t_1 < t_2) \). It is this feature that produces the Mott mid-gap pole at \( \omega = 0 \). Additional structure in the Hubbard bands merely gives rise to transient structure in the \( t_n \) for small \( n \) but importantly the parity of the alternation, \( t_{2n-1}/t_{2n} < 1 \), is preserved for all \( n \) [see Fig. 2(b)].

The SSH model in its topological phase (Eq. 2 with \( t_n \) given by Eq. 3 for all \( n \geq 1 \)) hosts an exponentially-localized boundary zero-mode (panel (c)). Right panels show the metallic FL (\( U/t = 3 \), \( D = 3 \): the low-energy \( \omega^* \) pseudogap in \( \text{Im}\Sigma(\omega) \) produces a generalized SSH chain with \( 1/n \) decay, in the trivial phase.

Metallic FL phase.—For \( U < U_c \), Eq. 1 describes a correlated metal, with low-energy FL properties characterized by a quadratic dependence of the self-energy, \( -\text{Im}\Sigma(\omega \to 0) \sim (\omega/Z)^2 \), in terms of the quasiparticle weight \( Z \). In Fig. 2(d) we plot the \( T = 0 \) self-energy deep in the FL phase, obtained by NRG-DMFT for \( U/t = 3 \). We obtain a distinctive form for the auxiliary chain hopping parameters from the continued fraction expansion,
arising due to the low-energy pseudogap in \( \text{Im} \Sigma(\omega) \),

\[
t_n^2 \approx \frac{nZ \gg 1}{D^2/4} \left[ 1 - \frac{r}{n+d}(-1)^n \right] \quad : \text{FL} \quad (4)
\]

where \( r = 2 \) is the exponent of the low-energy spectral power-law, and \( d \sim 1/Z \). Eq. 2 with hopping parameters \( t_n \) given by Eq. 4 generalizes the standard hard-gapped SSH model to the pseudogapped case: the alternating sequence of \( t_n \) again has a definite parity, but with a decaying \( 1/n \) envelope. Since \( t_{2n-1}/t_{2n} > 1 \) for all \( n \) (the chain starting this time from a strong bond), the analogous SSH model would be in its trivial phase; likewise here, the FL phase of the Hubbard model may be regarded as trivial. There is no localized boundary state of the auxiliary chain in the FL phase.

**Vicinity of transition.**—Deep in either MI or FL phases of the Hubbard model, the auxiliary chains are of generalized SSH model type, with the MI being topologically nontrivial. A robust and exponentially-localized zero-energy state lives on the boundary between the auxiliary and physical systems throughout the MI phase, corresponding to the Mott pole. However, richer physics is observed on approaching the Mott transition from the FL phase. In particular, the Mott transition occurs without bulk gap closing of the Hubbard bands (unusual for a topological phase transition). What is the mechanism for the transition between the trivial FL and the topological MI in terms of the auxiliary chains?

In the vicinity of the transition on the FL side, the self-energy develops a preformed gap, inside which are peaks located at \( \pm \omega_p \) with \( \omega_p \propto t \sqrt{Z} \), while quadratic ‘pseudogap’ behaviour sets in on the lowest energy scales \( |\omega| \ll \omega_p \) [7–9]. The transition corresponds to \( Z \to 0 \). Before performing the exact mapping \( \Sigma(\omega) \to \{ t_n \} \) numerically, we consider the evolution of chain parameters for a simpler toy system mimicking the Mott transition: two mid-gap spectral poles merging to zero.

To do this, we consider the general problem of determining the chain parameters \( t_n \) for a composite spectrum \( A(\omega) = \frac{1}{N} \sum_i w_i A_i(\omega) \), with \( N = \sum_i w_i \). Although spectral elements are simply additive, the composition rule for the \( t_n \) is highly non-linear. To make progress we note that spectral moments are additive, \( \mu_k = \frac{1}{N} \sum_i w_i \mu_i,k \) with \( \mu_i,k = \int d\omega \omega^k A_i(\omega) \), and use the moment expansion [51] of the chain parameters \( t_n^2 = X_n(n) \), where

\[
X_k(n) = \frac{X_k(n-1)}{t_{n-1}^2} - \frac{X_{k-1}(n-2)}{t_{n-2}^2}, \quad (5)
\]

with \( X_k(0) = \mu_{2k} \), \( X_k(-1) = 0 \) and \( t_{-1}^2 = t_0^2 = 1 \).

Analysis of the equations shows that adding a zero-energy pole to the boundary spectral function of the SSH model in the trivial phase flips the parity of the corresponding \( t_n \) (the first coupling of the chain swaps from a strong to a weak bond), yielding the topological SSH model, Eq. 3, as expected. What change in \( t_n \) results from adding two poles at \( \pm \omega_p \) to the trivial SSH spectrum, as depicted in Fig. 3(a)?

Figs. 3 (c,d) show the chain parameters \( t_n \) for \( \omega_p/D = 10^{-2} \) and \( 10^{-4} \). At large \( n \), the chain remains in the trivial SSH phase. However, a domain wall appears at \( n_{dw} \) where the parity of the alternation flips: the chain for \( 1 < n < n_{dw} \) is therefore in the topological phase of the SSH model (starting at \( n = 1 \) from a weak bond). This produces two localized states—one at the boundary (\( n = 1 \)), and the other pinned at the domain wall (\( n = n_{dw} \)), which hybridize and gap out to produce two states at energies \( \pm \omega_p \). Since these are topological states and exponentially localized, the hybridization is exponentially small in the real-space separation between them along the chain, and we find \( \omega_p \sim D \exp(-n_{dw} \delta/D) \).

This physical picture is confirmed by examining the exact eigenstates \( \psi_p \) with energy \( \omega_p \) satisfying \( H_{\text{aux}} \psi_p = \omega_p \psi_p \), plotted in panels (e,f).

The Mott transition as \( U \to U_c^- \) is characterized by \( \omega_p \to 0 \). In terms of the auxiliary chain, a pair of topological defects forms at the boundary when deep in the FL phase. One of these separates and moves down the chain as the transition is approached. As \( U \to U_c^- \) then \( \omega_p \to 0 \), and \( n_{dw} \to \infty \). At the transition itself, the two poles coalesce into the single Mott pole, and the chain is left with a single topological defect state at the boundary.

This mechanism is reminiscent of the vortex-pair dissociation in the Kosterlitz-Thouless transition [52]. The topological transition occurs without bulk gap closing.

The behaviour of the auxiliary chains for the actual Hubbard model is of course more complex than that of
the above toy model. In particular, the true self-energy \( \Sigma(\omega) \) is not completely hard-gapped in the FL phase, but features a low-energy quadratic pseudogap. Including this leads to alternating \( t_n \) with a \( 1/n \) envelope as per Eq. 4. Another key difference is that the peaks in the self-energy close to the transition are not delta-functions but have finite width. For the auxiliary chains, these peaks can be viewed as narrow bands of hybridizing topological states produced by a periodic structure of domain walls, as shown in the Supplementary Material [50]. One therefore expects a beating pattern in the chain parameters.

All these expected features are seen in the exact results for the self-energy and corresponding chain parameters close to the transition, shown in Fig. 4. In particular, the chains start from a weak bond (giving a localized boundary state); the position of the first domain wall moves to larger distances as \( \omega_p \) becomes smaller nearer the transition; the period of the beating becomes longer as the self-energy peaks become sharper; and the alternation in \( t_n \) attenuates as \( 1/n \) at long distances.

Combining these insights, we propose a simple toy model that approximates all of the qualitative features of the true lattice self-energy throughout the FL phase:

\[
I_{n}^2 = \frac{D^2}{4} \left[ 1 - \frac{2}{n + d} (-1)^n \right] \times [1 - \beta \cos(2\pi n/\lambda + \phi)] . \tag{6}
\]

A representative example is shown in Fig. 5(a), where we have fit the parameters of Eq. 6 to best match \( \Sigma(\omega) \) from NRG-DMFT [panel (c)] with \( \Delta_0(\omega) \) of the toy model [panel (b)]. The transition is approached as \( \lambda, d \to \infty \).

**Topological invariant.** – A recent paper by Logan and Galpin [9] shows for the Hubbard model Eq. 1 at \( T = 0 \) that the Luttinger integral takes distinct constant values in the FL and MI phases,

\[
I_L = \frac{2}{\pi} \text{Im} \int_{-\infty}^{0} d\omega G(\omega) \frac{d\Sigma(\omega)}{d\omega} = \begin{cases} 0 & : \text{FL} , \\ 1 & : \text{MI} \end{cases} \tag{T}
\]

The finite value of \( I_L \) for the generic MI [53] can be traced to the Mott pole, which we identified in this work as the topological feature of the MI. Indeed, it has been suggested that violation of Luttinger’s theorem implies topological order [34–39, 42]. Since the evolution of the self-energy with interaction strength drives the Mott transition, the Luttinger integral is a natural quantity to characterize the distinct topology of the FL and MI phases, and may be regarded as a topological invariant.

**Conclusions.** – We present an interpretation of the classic Mott transition in the infinite-dimensional one-band Hubbard model as a topological phase transition. The lattice self-energy, determined here by NRG-DMFT, is mapped to an auxiliary tight-binding chain, which is found to be of generalized SSH model type. The MI is the topological phase, with a boundary-localized zero-energy state corresponding to the Mott pole. The transition from FL to MI involves domain wall dissociation.

We argue that any system with a zero-pole in its local self-energy may be similarly regarded as topological. It would be interesting to explore the mapping away from half-filling and at finite temperature, as well as the time-dependence after a quench. The analysis could also be extended to multi-band models, where the auxiliary chains become multi-legged ladders. We speculate that a superconducting Hubbard model may map to auxiliary Ki-
taev chains involving Majoranas. For a fully momentum-dependent self-energy of a $D$-dimensional lattice, the mapping generalizes to an auxiliary lattice in $D + 1$ dimensions; for a MI, the auxiliary lattice may be a topological insulator with a localized boundary state.

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Results presented are insensitive to the choice of $D$. See Supplementary Material.

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$I_L = 1$ throughout the MI phase at $T = 0$ except at exact particle-hole symmetry [9], which appears to be a pathological point (possibly due to the order of limits for particle-hole symmetry-breaking and temperature).
The Mott transition as a topological phase transition:
Supplementary Material

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This Supplementary Material consists of the following. In section S-1 we provide technical details of the continued fraction expansion (CFE) of the Hubbard model self-energy and discuss the analytic structure of auxiliary chain correlation functions. In section S-2 we demonstrate the veracity of the obtained auxiliary chain hopping parameters \( \{t_n\} \), by reproducing the input. In section S-3 we discuss the ‘moment expansion’ technique, and its advantages and drawbacks in the context of the current work. In section S-4 we provide additional analysis of the role of the mid-gap peaks on the chain structure. In section S-5 we discuss an alternative topological signature of the auxiliary chains based on boundary conductance arguments. Section S-6 contains technical details of the NRG and DMFT calculations.

S-1. AUXILIARY CHAIN CORRELATION FUNCTIONS

In this section we discuss technical details of the CFE for the mapping of the self-energy \( \Sigma(\omega) \) to the auxiliary chain parameters \( \{t_n\} \), which constitute a kind of ‘genetic code’ describing the role of electronic correlations in these systems. We also examine the mathematical structure of the auxiliary hybridization functions \( \Delta_n(\omega) \).

The local lattice self-energy \( \Sigma(\omega) \) as a function of real frequency \( \omega \), is the input for the calculations, and is assumed to be known. In the present work we use NRG-DMFT to obtain it at \( T = 0 \) (see Sec. S-6), but in principle any suitable method can be used. The self-energy is identified with a hybridization \( \Delta_n(\omega) \) between the physical lattice degrees of freedom and fictitious auxiliary degrees of freedom which provide the same (single-particle) dynamics, \( \Delta_n(\omega) = \Sigma(\omega) \). Furthermore, this hybridization can be written in terms of the boundary Green’s function of the free auxiliary system – here a semi-infinite tight-binding chain given by Eq. 2 of the main paper. We write \( \Delta_n(\omega) = V^2 G_1(\omega) \), with \( V \) the tunneling matrix element between the physical lattice sites and the auxiliary chains appearing in \( H_{\text{hyb}} \), and \( G_1(\omega) = \langle f_{\sigma,1}^\dagger f_{\sigma,1}\rangle \) is the retarded Green’s function (the prime denotes the isolated \( H_{\text{aux}} \)). We define \( \Delta_0(\omega) = -\frac{1}{\pi} \text{Im} \Delta_n(\omega) \), such that \( \int d\omega \Delta_0(\omega) = V^2 \).

S-1.1. Continued fraction expansion of self-energy

The boundary Green’s function of the auxiliary chain can be expressed as \( G_1(\omega) = 1/(\omega^+ - \Delta_1(\omega)) \) where \( \omega^+ = \omega + i0^+ \) and \( \Delta_1(\omega) \) is the hybridization to the rest of the chain. \( \Delta_1(\omega) = t_0^2 \tilde{G}_2(\omega) \) can also be expressed in terms of a Green’s function. In this case, it is the boundary Green’s function of a chain starting at site \( n = 2 \) (i.e., the Green’s function at the end of the auxiliary chain with site 1 removed). Following the same logic recursively, we obtain \( \tilde{G}_n(\omega) = 1/(\omega^+ - \Delta_n(\omega)) \) for \( n \geq 1 \), where \( \Delta_n(\omega) = t_n^2 \tilde{G}_{n+1}(\omega) \). Here, \( \tilde{G}_m(\omega) = \langle \langle f_{\sigma,m}^\dagger f_{\sigma,m}\rangle \rangle \) is the Green’s function of the auxiliary chain at site \( m \) with all sites \( < m \) removed. We therefore obtain the continued fraction expansion,

\[
\Delta_0(\omega) = \frac{V^2}{\omega^+ - \frac{t_1^2}{\omega^+ - \frac{t_2^2}{\omega^+ - \ddots}}}.
\]

Starting from \( \Delta_0(\omega) = \Sigma(\omega) \), and using \( \int d\omega A_n(\omega) \equiv -\frac{1}{\pi} \int d\omega \text{Im} \Delta_n(\omega) = t_n^2 \), one can recursively determine all \( t_n \). Although in practice the recursive procedure is stopped after a finite number of iterations, \( N \), note that the \( t_n \) determined \textit{en route} are (numerically) exact and are not affected by truncating the sequence at finite \( N \) (this is in contrast to methods involving discretization of the spectrum, or the moment expansion discussed below which is strongly nonlinear). For large enough \( N \), the asymptotic properties of the chain parameters can be identified, and can be analytically continued, using a chain ‘terminator’. We observe that thousands of sites of the auxiliary chain must typically be determined to capture low-energy features in the FL phase. In the MI phase, shorter chains of a few hundred sites are usually sufficient to identify the asymptotic chain properties. We emphasize that in all cases an accurate representation of the self-energy requires long (preferably analytically continued) auxiliary chains. Representations involving only a few ‘ghost’ sites are not adequate.

Finally, we point out that accurate self-energies with high resolution in frequency must be used to recover the auxiliary chain properties discussed in this work.

S-1.2. Auxiliary chain representation of a Fermi liquid (FL)

In the FL phase, the technical complexity in determining \( \{t_n\} \) numerically is due to the low energy form of the
(input) self-energy. In this case,
\[ \Delta_0(\omega) \sim a_0\omega + ib_0\omega^2 \quad (a_0, b_0 < 0) . \]

**Step 1:** Calculation of \( \Delta_1(\omega) : \)
\[ \Delta_1(\omega) = t_1^2\tilde{G}_2(\omega) = \omega^+ - 1/G_1(\omega). \]
Since both the real and imaginary parts of \( G_1(\omega) \) is vanishingly small as \( \omega \to 0 \) and is equal to zero at \( \omega = 0 \), this leads to a non-analyticity in \( \Delta_1(\omega = 0) \) and hence a singular part in the corresponding Green’s function \( \tilde{G}_2(\omega) \).

We write \( \tilde{G}_2(\omega) = \tilde{G}_2^{reg}(\omega) + \tilde{G}_2^{sing}(\omega) \), where \( \tilde{G}_2^{reg}(\omega) \) represents the regular (continuum) part, and \( \tilde{G}_2^{sing}(\omega) \) represents the singular part. More precisely,
\[ \Delta_1(\omega = 0) = \omega^+ - \frac{t_1^2}{a_0\omega + ib_0\omega^2} = \omega^+ - \frac{t_1^2}{a_0} \left[ \frac{1}{\omega^+} + \frac{ib_0}{a_0 + ib_0\omega} \right]. \]
Therefore we identify
\[ \Delta_1^{reg}(\omega \to 0) = \omega + \frac{t_1^2\omega + ib_0\omega^2}{a_0(a_0^2 + b_0^2\omega^2)} + i\frac{t_1^2b_0}{a_0^2 + b_0^2\omega^2}, \]
such that,
\[ \Delta_1(\omega \to 0) = \Delta_1^{reg}(0) - \frac{t_1^2}{a_0\omega^+}. \]

The second term in Eq. (2) corresponds to a pole in the imaginary part concomitant with a diverging real part of \( \Delta_1(\omega) \) at \( \omega = 0 \). Furthermore, this pole resides on top of a background function, \( \Delta_1^{reg}(\omega) \), such that \( \Delta_1^{reg}(0) = \beta \). The residue of this pole is \( \alpha_1 = \frac{t_1^2}{|a_0|} \). To fix \( t_1^2 \) we use the spectral normalization,
\[ t_1^2 = \int \Delta_1^{reg}(\omega)d\omega + \alpha_1 , \]

**Step 2:** The low energy spectral behavior of \( \Delta_2(\omega) \) is,
\[ \Delta_2(\omega) = \omega - \frac{\omega t_1^2}{\omega \Delta_1^{reg}(\omega) + \alpha_1}. \]
Evaluating the imaginary part,
\[ \text{Im} \Delta_2(\omega) = -\omega t_1^2 \text{Im} \frac{1}{\omega \Delta_1^{reg}(\omega) + \alpha_1} = \frac{2i t_1^2 \text{Im} \Delta_1^{reg}}{(\omega \text{Re}(\Delta_1^{reg}) + \alpha_1)^2 + (\omega \text{Im}(\Delta_1^{reg}))^2}. \]

Substituting the respective low energy dependencies of \( \Delta_1^{reg}(\omega) \) we find that \( \text{Im} \Delta_2(\omega) \sim 0 \) for \( \omega \to 0 \). Similarly, if we evaluate \( \text{Re} \Delta_2(\omega \to 0) \) it follows from the presence of a non-zero \( \alpha_1 \) that \( \text{Re} \Delta_2(\omega \to 0) \sim 0 \). Just like a Fermi liquid. The advantage of separating the regular and singular part of the odd-site chain hybridizations is thus clear from the structure of Eq. (5), where the information about the underlying pole from the previous iteration is embedded via its weight, and allows us to deal with a regular function numerically.

Based on the above, it is clear that at every odd recursion step, \( \Delta_{2n+1}(\omega) \) will have a pole structure similar to \( \Delta_1(\omega) \) with a pole weight \( \alpha_{2n+1} = \frac{t_2^2}{|a_{2n}|} \) and subsequently the FL character will follow for every even numbered site in the chain, namely, \( \Delta_{2n}(\omega) \). In summary, the following recursion relations describe the flow of the low-energy expansion coefficients,
\[ \Delta_{2n}(\omega \to 0) = a_{2n}\omega + ib_{2n}\omega^2 \quad (a_{2n}, b_{2n} < 0) , \]
\[ \Delta_{2n+1}(\omega \to 0) = \frac{\alpha_{2n+1}}{\omega^+} + i\beta_{2n+1}, \]
\[ a_{2n} = 1 - \frac{t_{2n}^2}{\alpha_{2n-1}} \quad ; \quad b_{2n} = \frac{t_{2n}^2\beta_{2n-1}}{\alpha_{2n-1}}, \]
\[ \alpha_{2n+1} = \frac{t_{2n}^2}{|a_{2n}|} \quad ; \quad \beta_{2n+1} = \frac{t_{2n}^2b_{2n}}{a_{2n}^2}. \]

The asymptotic properties of the \( \Delta_n(\omega) \) are therefore completely determined by the initialized values \( a_0, b_0 \) and the \( \{t_n\} \) determined by the above CFE.

Note that the above analytic structure is a fingerprint of the FL phase: all \( \text{Im} \Delta_n(\omega) \) for even \( n \) have low-energy quadratic behaviour, while all odd \( n \) functions have zero-energy poles.

On the practical level of the numerical calculations, for every odd iteration we cut the singular pole feature from \( A_{2n+1}(\omega) \), perform a Kramers-Kröning transformation to obtain the regular real part, and hence \( \Delta_n^{reg}(\omega) \). The even or odd \( t_n \) are subsequently evaluated at each iteration from the normalisation of \( A_n(\omega) \) as above.

**S-1.3. Auxiliary chain representation of the Mott insulator (MI)**

For a MI, \( \Delta_0(\omega) \) is hard-gapped for \( \omega \in [-\delta : \delta] \), where \( 2\delta \) is the size of the Mott gap. Inside the gap resides a zero-energy pole (the ‘Mott pole’), such that \( \Delta_0(\omega \to 0) = \frac{\alpha_1}{\omega} \). Based on the analysis for the FL self-energy in the previous subsection, we readily observe that in the MI case, the role of odd and even chain sites is now interchanged. In addition, we note that \( \beta = 0 \) for all (even) \( n \) for the MI because the pole is sitting inside the Mott gap and the \( b \) coefficients are also zero for all odd \( n \). The low-energy asymptotic behaviour and coefficient
 recursion (for $n \geq 1$) follows,
\[ \Delta_{2n-1}(\omega \to 0) = a_{2n-1}\omega , \quad (10) \]
\[ \Delta_{2n}(\omega \to 0) = \frac{\alpha_{2n}}{\omega + i\delta} , \quad (11) \]
\[ a_{2n-1} = 1 - \frac{t_{2n-2}^2}{\alpha_{2n-2}} , \quad b_{2n-1} = 0 , \quad (12) \]
\[ \alpha_{2n} = \frac{t_{2n-1}^2}{|a_{2n-1}|} , \quad \beta_{2n} = 0 . \quad (13) \]

Thus the pole structure of the MI $\Delta_n(\omega)$ is reversed with respect to the FL. Importantly, the imaginary part of the hybridizations $\Delta_n(\omega)$ is hard gapped for all $n$, but contains a mid-gap zero energy pole for all even $n$ (only).

S-2. Self-Energies Reproduced from Numerically Evaluated $t_n$ Sequences

Using the the semi-analytic procedure described in section S-1 we obtain a sequence of the auxiliary chain hopping parameters, $\{t_n\}$. We terminate the recursion after a finite number of steps, $N$ (typically a few thousand). As a check that the derived auxiliary chain does faithfully describe the input self-energy, we numerically evaluate the continued fraction Eq. 1. In practice, we use $\omega^+ = \omega + i\delta$ with some small but finite $\delta > 0$. We also analytically continue the chain beyond step $N$ for a further $10^6$ sites using the identified asymptotic behaviour. The form of this ‘terminator’ is given by Eq. 4 or Eq. 5 of the main text.

In Figure 1 we compare $-\text{Im }\Delta_0(\omega)$ from the CFE with the input $-\text{Im }\Sigma(\omega)$ for different interaction strengths $U$. As can be seen the $t_n$ sequence obtained, excellently reproduces the original Hubbard model self-energy, $\Sigma(\omega)$. Any deviations at very small $\omega$ are due to the finite $\delta$ used, and can be systematically pushed to lower $\omega$ by using a smaller $\delta$ together with a longer chain.

S-3. Moment Expansion Technique

Given a spectral function, the spectral moments are determined from $\mu_n = \int_{-\infty}^{\infty} \omega^n A(\omega) d\omega$ where $D$ is the half bandwidth. $\mu_0 = 1$ for a normalised spectral function. Furthermore, for a symmetric spectrum $A(\omega) = A(-\omega)$, only the even moments survive, $\mu_{2n} = 0$.

For more details the reader is referred to Ref. 1 and references therein, where this scheme is discussed on more general grounds. Here we outline only the main equations that were utilised to generate the hopping parameters evaluated in Figure 3 of the main text. Also, here we discuss only the case of particle-hole symmetric spectral function.

As described in Eq. 5 of the main text, given a set of spectral moments, $\{\mu_0, \mu_2, \mu_4, \ldots, \mu_{2N}\}$ it is possible to generate the first $N$ coefficients in the set $\{t_n\}$.

However, it should be noted that while this recursive scheme appears straightforward, it is well known in the literature\cite{footnote1, footnote2} that determination of the CFE coefficients via moment expansion is numerically very unstable. The spectral moments essentially must be known exactly (obtaining them from numerical integration of the raw spectrum is not sufficient). Furthermore, the recursive calculation must be performed on the computer with arbitrary precision numerics (the scheme breaks down after about 15 steps even with analytically known moments when using standard double-precision numerics).\cite{footnote1} For our toy models discussed in the main text, where the spectral moments are known exactly, and using arbitrary precision numerics, we could extract reliably the first 200
chain coefficients before the calculation breaks down and become non-physical.

Therefore, while seemingly appealing, the moment expansion method is not in general of use for determining the auxiliary chain coefficients for the self-energy. We use it for Fig. 3 because we can treat poles and hard gaps cleanly.

S-4. MID-GAP PEAKS AS BANDS OF HYBRIDIZING TOPOLOGICAL STATES

In the main text of the paper, we discuss how the trivial SSH model with two additional mid-gap delta-functions at energies ±ωp can be interpreted in terms of domain-wall physics on the chain. Using the moment expansion technique discussed above, we found that localized states on the boundary and pinned to the domain wall hybridize through the intervening gapped SSH medium, lifting the degeneracy. Since the topological states are exponentially well-localized, we argued on physical grounds (and also showed by explicit calculation in Fig. 3b) that ωp ∼ D exp(−n_{dw}δ/D), where 2D is the full bandwidth, 2δ is the SSH full gap width, and n_{dw} is the position of the domain wall (real-space separation on the chain between the localized states).

In this section, we generalize the above picture to the situation where the mid-gap peaks have finite width Δp, rather than treating simply delta-function spectral poles. This is of relevance to the FL phase of the Hubbard model, since the self-energy peaks sitting inside the preformed gap near the Mott transition are sharp, but not poles.

We follow a similar strategy here to that in the main text. Specifically, we consider a trivial SSH model with bandwidth 2D and gap 2δ as before, but now insert another trivial SSH model inside the gap, with bandwidth 2Dp and gap 2δp, where Dp < δ and the mid-gap peaks are then of half-width Δp = 1/2(Dp + δp). The centre of the peak positions are at ωp = 1/2(Dp + δp). The setup is illustrated in Fig. 2(a) for D = 1 and δ = 0.2. Note that the peaks become delta-functions as Δp → 0, and we recover the results of the main text.

We again use the moment expansion technique to derive the chain coefficients {tn} for such a setup. The results are shown in Figs. 2(b,c) for common Dp = 10^{-2}, varying Δp = 10^{-3} [panel (b)] and 10^{-5} [panel (c)]. The general structure is that of the usual SSH chain, starting at n = 1 from a weak bond (indicating the existence of a localized boundary state), but also featuring domain walls. Unlike the case of mid-gap spectral delta-functions, now we have several domain walls. We denote the chain position of domain wall l as xl, with l = 1 being at the boundary, x1 = 1.

In fact, the domain walls arise with definite periodicity on the chain. Importantly, the first domain wall away from the boundary, at x2, is fixed by ωp, and therefore does note change as we vary only Δp in Fig. 2(b,c). As before, ωp ∼ D exp(−n_{1}δ/D), where n_{1} = x_{2} − x_{1}. The separation between the next two domain walls is n_{2} = x_{3} − x_{2}, and controls the width of the mid-gap peaks, Δp ∼ D exp(−n_{2}δ/D), as shown in Fig. 2(d). This structure then repeats periodically: x_{2k} − x_{2k−1} = n_{1} and x_{2k+1} − x_{2k} = n_{2} for all k ≥ 1.

Such a chain gives rise to a narrow band of hybridizing topological states, which are precisely the mid-gap peaks. Denoting a given topological localized zero-energy state ψ_{l} in an SSH chain with a single domain wall at x_{1} as |ψ_{l}⟩, we can formulate an effective model for the mid-gap states including through-chain hybridization, viz:

\[ H_{\text{eff}} = \sum_{l=1}^{\infty} \omega_{p}|\psi_{2l−1}⟩⟨\psi_{2l}| + Δ_{p}|\psi_{2l}⟩⟨\psi_{2l+1}| + \text{H.c.} , \quad (14) \]
which is again of SSH form. Since $n_1 < n_2$, we have $\omega_p > \Delta_p$, and so the mid-gap peaks can be viewed as a trivial band of hybridizing topological states.

Our conclusion is that finite self-energy peak width must give rise to a beating pattern of the SSH chain coefficients. This is confirmed in the full numerical calculations of $\{t_n\}$ for the true lattice self-energy of the Hubbard model in the FL phase near the transition, Fig. 4 of the main text.

In particular, note that as the peaks sharpen into poles $\Delta_p \to 0$, the period $n_2$ grows and diverges, leaving localized states at $n = 1$ and $n = n_1$ only, as per Fig. 3 of the main text. But, as the Mott transition is approached $U \to U_c^-$, the peaks not only sharpen but also move to lower energy and coalesce, $\omega_p \to 0$. This corresponds to diverging $n_1$. At the transition, and throughout the MI phase, we are then left with a single localized boundary state at $n = 1$, and the chain becomes the regular SSH chain in the topological phase. This is all achieved without bulk gap closing.

S-5. BOUNDARY CONDUCTANCE OF THE AUXILIARY CHAIN

A further signature of the topological nature of the Mott insulator self-energy, is a quantized fictitious $T = 0$ ‘conductance’ through the end of the auxiliary chain $G_c/[2e^2/h] = \pi\Gamma A_{11}^{aux}(\omega = 0) = 1$ (where $\Gamma$ is the hybridization to fictitious electrodes, and $A_{11}^{aux}$ is the spectral function at the end of the electrode-coupled auxiliary chain). By contrast with the Mott insulator, the fictitious $T = 0$ conductance through the end of the auxiliary chain precisely vanishes in the Fermi liquid phase, $G_c/[2e^2/h] = \pi\Gamma A_{11}^{aux}(\omega = 0) = 0$.

S-6. DETAILS OF NRG-DMFT CALCULATIONS

In this work, we solve the infinite-dimensional one-band Hubbard model on the Bethe lattice (Eq. 1 of the main text) numerically exactly at temperature $T = 0$, using dynamical mean field theory (DMFT), with Wilson’s numerical renormalization group (NRG) method as the underlying quantum impurity solver. NRG has the clear advantage over other impurity solvers (for this class of few-channel problems) in that real-frequency correlation functions can be obtained down to arbitrarily low energies, at any temperature including $T = 0$, for any type of impurity interaction and strength. This is made possible by several important recent technical advances over Wilson’s original formulation of the method.

For the purposes of the CFE of the self-energy, high-quality data for the self-energy are required. For the calculations presented in this paper, we use NRG discretization parameter $\Lambda = 2$, retain $N_z = 6000$ states at each iteration, and average the results of $N_z = 20$ different bath discretizations. Total charge and spin projection quantum numbers are implemented. Correlation functions were obtained using the full density matrix method utilizing the complete Anders-Schiller basis. For converged solutions on the lattice, typically 10–20 DMFT iterations are required.

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