Supplemental Material: Terminable Transitions in a Topological Fermionic Ladder

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A. Extrapolating correlation lengths and gaps

To find the phase transition line where an excitation gap closes, we can compute the gap directly on finite systems of length L and extrapolate to the infinite limit in L^{-1}. This can be resolved by quantum number: $\Delta_{\text{spin}} = E_0\,(S=1, N=L) - E_0\,(S=0, N=L)$ defines the spin gap, $\Delta_{\text{charge}} = E_0\,(S=1/2, N=L+1) - E_0\,(S=0, N=L)$ defines the charge gap, while $\Delta_{\text{neutral}} = E_1\,(S=0, N=L) - E_0\,(S=0, N=L)$ defines the neutral gap, whereby we label E_0 (E_1) the lowest (second lowest) eigenenergy in a given sector.

The result of this process is shown in Fig. S1 above the termination point, clearly showing that all gaps remain finite.

Another possibility is to compute the inverse correlation length ξ^{-1} for the infinite system, which also goes to zero at the gap closure. The correlation length is in this case obtained from the dominant eigenvalue of the transfer matrix at a fixed bond dimension χ [1–3] and can also be resolved by the same quantum numbers as above. (Note that the main text shows the neutral correlation length measured in sites rather than unit cells).

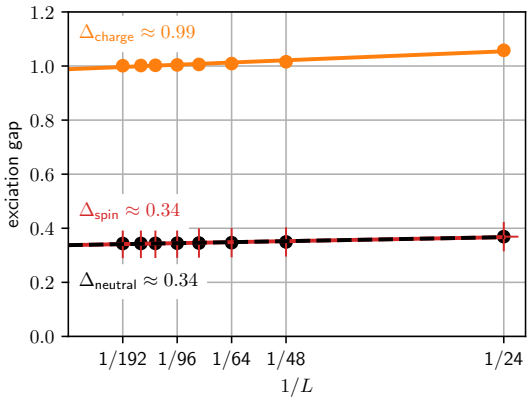

FIG. S1. Gap extrapolation for $U = V_\perp = 4$ (minimal model) for systems of length L (with $L/2$ rungs). Energies are obtained using DMRG for finite ladders with a trivial cut (unlike Fig.5).

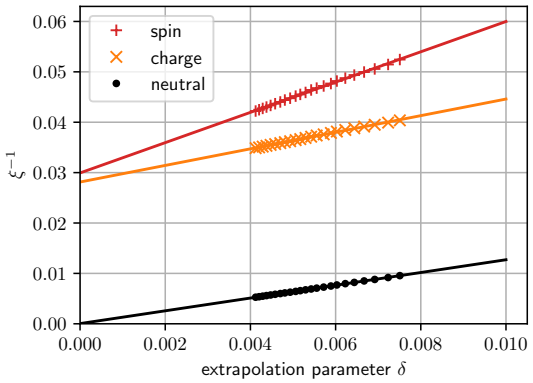

FIG. S2. Extrapolation of the inverse correlation length ξ^{-1} (measured in sites and using the trivial cut) for $U = V_\perp = 2$ (minimal model), resolved by the quantum number. The results were obtained using VUMPS for the infinite system. The extrapolation parameter δ is defined as in Ref. 2.

One can use different extrapolation parameters δ that measure the closeness to the exact ground state (e.g. the inverse bond dimension χ^{-1}). Here, we follow Ref. 2, where a parameter was found with which $\xi^{-1}\,(\delta)$ generally becomes linear.

Figure S2 shows this procedure below the termination point. We find that the neutral correlation length vanishes, while charge and spin gaps remain open.

B. Microscopic analysis for the role of the operator O_j

In this section, we derive an understanding of the singlet density operator O_j in terms of the subband picture of the ladder.

We repeat the Hamiltonian of the minimal model in the subband basis introduced in the main text:

$$H = -t_\parallel \sum_{j,k_y,\sigma} (c^\dagger_{j,k_y,\sigma} c_{j+1,k_y,\sigma} + h.c.) - t_\perp \sum_j [n_{j,\pi} - n_{j,0}] + U/2 \sum_j [\Delta n_{j,\pi} + \Delta n_{j,0}]^2 - (U - V_\perp) H_{\text{res}}. \quad \text{(S1)}$$

Rewriting O_j in the same basis, we obtain:

$$O_j = -c^\dagger_{j,0,\uparrow}c^\dagger_{j,0,\downarrow}c_{j,\pi,\uparrow}c_{j,\pi,\downarrow} + H.c. \tag{S2}$$

We see that O_j describes the hopping of fermion pairs between the two subbands and can be used to characterize the strength of virtual scattering that violates the subband U(1) symmetry. Since the particle numbers in the subbands are conserved for $U = V_\perp$, the hopping between them must also vanish along this line: $\langle O_j\rangle = 0$.

To understand that $\langle O_j\rangle$ and $U - V_\perp$ have the same sign, we note that the residual term is given by $H_{\rm res} = \sum_j O_j/2 + ...$, where the subband U(1) preserving terms have been neglected. Therefore, $-(U - V_\perp)\langle O_j\rangle < 0$ is expected to minimize the energy.

Similar to the above energy minimization argument for $\langle O_j\rangle$, we can argue that if there are subband U(1) violating terms breaking time-reversal symmetry (TRS) $\propto \sum_j e^{i\alpha}c^\dagger_{j,0,\uparrow}c^\dagger_{j,0,\downarrow}c_{j,\pi,\uparrow}c_{j,\pi,\downarrow} + H.c.$, the subband U(1) point can be avoided along a path connecting D-Mott to S-Mott by tuning α from 0 to π. This indicates that TRS plays an important role for the existence of a transition. This analysis is closely related to the bosonization analysis of discreetness of locking values in the main text.

As shown in the main text, the ground state $\langle n_{j,\pi}\rangle = 0$ and $\langle n_{j,0}\rangle = 2$ for $U = V_\perp \gtrsim 3.4$ can be written as rung bisinglet $\prod_j 1/\sqrt{2}(\Delta^\dagger_{{\rm S}j} + \Delta^\dagger_{{\rm D}j})|\Omega\rangle$. Recall from the main text that the model wave function of D- and S-Mott ($|{\rm D}\rangle = \prod_j \Delta^\dagger_{{\rm D}j}|\Omega\rangle$ and $|{\rm S}\rangle = \prod_j \Delta^\dagger_{{\rm S}j}|\Omega\rangle$) consists rungs of two eigenstates of O operators. Consider O as an Ising field, the tendency to form rung bisinglet can be induced by transverse field, which is the counter part of the temperature in the quantum-classical analogy. This is one way to draw an analogy to the magnet picture of terminable first-order transition. However, with accidental symmetry or weak interaction, the analogues of magnetic ordering terms can vanish simultaneously (see the scaling dimension analysis in the main text) such that the transition is not first order as the magnetic picture.

C. Effective band structure

In this section, we offer a perspective on the termination of the phase transition for the minimal model from the effective band structure.

The criticality at $U = V_\perp$ and its termination is related to the subband occupation ratio $\langle n_{j,\pi}\rangle / \langle n_{j,0}\rangle$ (which is not dependent on j in the homogeneous case). When this filling ratio is fractional, according to Lieb-Schultz-Mattis theorem [4, 5], the system must be gapless, unless there is a spontaneous breaking of translational symmetry resulting in a degenerate ground state.

Introducing the single-particle retarded Green's function

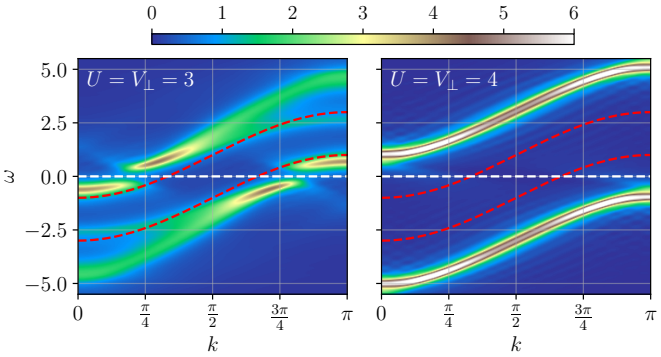

FIG. S3. The spectral function Eq. (S5). Red dashed line: band structure of the noninteracting model; white dashed line: reference for $\omega = 0$. The results are obtained by a real-time evolution of Eq. (S3) to $t_{\rm max} = 20$ using infinite boundary conditions [6, 7].

$$G^{ll'}\left(t, |j - j'|\right) = -i\theta(t)\Big[\sum_\sigma \langle 0|e^{iHt}c^\dagger_{jl\sigma}e^{-iHt}c_{j'l'\sigma}|0\rangle + \sum_\sigma \langle 0|e^{-iHt}c_{jl\sigma}e^{iHt}c^\dagger_{j'l'\sigma}|0\rangle\Big] \tag{S3}$$

and its Fourier transform

$$G^{ll'}(\omega, k) = \sum_d e^{ikd}\int_{-\infty}^{\infty} dt\; e^{i\omega t}G^{ll'}(t, d), \tag{S4}$$

we can define the equivalent of the bandstructure in presence of interactions by the spectral function

$$S(\omega, k) = -\frac{1}{\pi}\sum_{l={\rm A,B}} {\rm Im}\; G^{ll}(\omega, k). \tag{S5}$$

This spectral function is displayed in Fig. S3. It reveals the two-subband structure of the ladder, whereby the lower subband has $k_y = 0$ and the upper subband has $k_y = \pi$. The parts of the subbands that lie below the Fermi edge $\omega = 0$ reflect $\langle n_{j,\pi}\rangle$ and $\langle n_{j,0}\rangle$ when integrated. In the noninteracting limit we have $\langle n_{j,\pi}\rangle / \langle n_{j,0}\rangle = 1/2$. Our calculations show that $\langle n_{j,\pi}\rangle / \langle n_{j,0}\rangle$ can change continuously along the line $U = V_\perp$. The effect of interactions is to increase the splitting of the subbands, so that for $U = V_\perp \gtrsim 3.4$, only the lower band is below the Fermi energy. This implies an integer filling $\langle n_{j,\pi}\rangle = 0$ and $\langle n_{j,0}\rangle = 2$ and the state effectively becomes a band insulator, where the two-band bosonization is no longer valid. This is why within the two-band bosonization, it is not clear that the two Mott regions can be adiabatically connected.

D. The bosonization of O_j

Here, we discuss the two-band bosonization of O_j. Recall that the definition is

$$O_j = -c^\dagger_{j,0,\uparrow}c^\dagger_{j,0,\downarrow}c_{j,\pi,\uparrow}c_{j,\pi,\downarrow} + H.c. \tag{S6}$$

In addition to the terms presented in the main text, we include oscillatory terms and discuss higher harmonics. Recall that the bosonization of fermion operators to the lowest harmonics is

$$c_{k_y,\sigma}(x_j) = \frac{\kappa_{k_y,\sigma}}{\sqrt{2\pi}} \sum_{\eta=-1,1} e^{i[\theta_{k_y,\sigma}+\eta(\phi_{k_y,\sigma}+k_{\mathrm{F},k_y,\sigma}x_j)]}. \tag{S7}$$

We insert Eq. (S7) into Eq. (S6) to obtain the lowest harmonics of the bosonization of O_j

$$\begin{aligned} O_j \propto & \cos(2\tilde{\theta}_{c,-})[\cos(2\tilde{\phi}_{s,-}) + \cos(2\tilde{\phi}_{s,+}) + \\ & \cos(2\tilde{\phi}_{c,+} + \sum_{\sigma,k_y} k_{\mathrm{F},k_y,\sigma}x_j) + \\ & \cos(2\tilde{\phi}_{c,-} + \sum_{\sigma}(k_{\mathrm{F},\pi,\sigma} - k_{\mathrm{F},0,\sigma})x_j) + \\ & \cos(\tilde{\phi}_{c,+} + \tilde{\phi}_{c,-} + \tilde{\phi}_{s,+} - \tilde{\phi}_{s,-} + \sum_{\sigma} k_{\mathrm{F},0,\sigma}x_j) + \\ & \cos(\tilde{\phi}_{c,+} - \tilde{\phi}_{c,-} + \tilde{\phi}_{s,+} + \tilde{\phi}_{s,-} + \sum_{\sigma} k_{\mathrm{F},\pi,\sigma}x_j) + ..., \end{aligned} \tag{S8}$$

where the higher harmonics are neglected. The coefficients of each term are neglected for simplicity. At half filling, $\sum_{\sigma,k_y} k_{\mathrm{F},k_y,\sigma} = 2\pi$, which can be set to be 0, as x_j are integer. For the Mott states, as well as the D-Mott/S-Mott transition (shown to be of Gaussian type, see below), $\tilde{\phi}_{c,+}$, $\tilde{\phi}_{s,-}$,$\tilde{\phi}_{s,+}$ are kept locked and can be set to zero for discussing expectation values or correlation function. So in this special case, we have

$$\begin{aligned} O_j \propto & \cos(2\tilde{\theta}_{c,-}) + \cos(2\tilde{\theta}_{c,-})[\cos(2\tilde{\phi}_{c,-} + 2\Delta k_{\mathrm{F}}x_j) + \\ & \cos(\tilde{\phi}_{c,-} + 2k_{\mathrm{F},0,\sigma}x_j) + \cos(\tilde{\phi}_{c,-} + 2k_{\mathrm{F},\pi,\sigma}x_j)], \end{aligned} \tag{S9}$$

where $\Delta k_{\mathrm{F}} = k_{\mathrm{F},0,\sigma} - k_{\mathrm{F},\pi,\sigma}$; for our model, $k_{\mathrm{F},k_y,\uparrow} = k_{\mathrm{F},k_y,\downarrow}$. The coefficient of each term is neglected for simplicity. These are only two values $\tilde{\theta}_{c,-}$ can be locked at if there is no explicit or spontaneous TRS breaking; this can be seen by evaluating TRS odd term $i(c^\dagger_{j,0,\uparrow}c^\dagger_{j,0,\downarrow}c_{j,\pi,\uparrow}c_{j,\pi,\downarrow} - h.c) \propto \sin(2\tilde{\theta}_{c,-})$. In fact, $\tilde{\theta}_{c,-} \to -\tilde{\theta}_{c,-}$ for time-reversal symmetry, thus $\cos(2\tilde{\theta}_{c,-} + \alpha)$ with generic α is forbidden to appear in a time-reversal symmetric Hamiltonian. The locking values are 0 and $\pi/2$ Thus, with TRS, the expected continuous transition within the 2-band effective theory is that $\tilde{\theta}_{c,-}$ becomes unlocked, indicating a Gaussian criticality. This is consistent with the microscopic argument of the TRS's role for the existence of the transition.

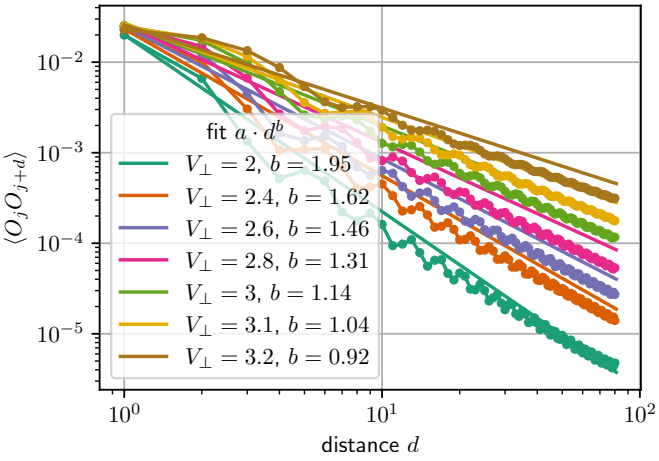

FIG. S4. Correlation function $\langle O_j O_{j+d}\rangle$ for $U = V_\perp$ for the minimal model obtained in the infinite system. The straight solid lines are references for the fitted slope of the data with the same color.

E. Correlations $\langle O_j O_{j+d}\rangle$ and Gaussian criticality

For the minimal model and $U = V_\perp \lesssim 3.4$, as pointed out in the main text, the field $\tilde{\theta}_{c,-}$. and its dual field $\tilde{\phi}_{c,-}$ is gapless and characterized by a Luttinger parameter K (Eq. (8)). Here we compute $\langle O_j O_{j+d}\rangle$ using Eq. (S9) of which each term gives an algebraic decay component.

$$\begin{aligned} \langle O_j O_{j+d}\rangle = & \frac{1}{|d|^{2/K}} + \frac{\cos(2k_{\mathrm{F},0,\sigma}d)}{|d|^{2/K+K/2}} + \frac{\cos(2k_{\mathrm{F},\pi,\sigma}d)}{|d|^{2/K+K/2}} + \\ & \frac{\cos(2\Delta k_{\mathrm{F}}d)}{|d|^{2/K+2K}} \end{aligned} \tag{S10}$$

The coefficient of each term is neglected for simplicity. We see that the leading term is non-oscillatory while subleading terms can be oscillatory.

The data of $\langle O_j O_{j+d}\rangle$ for various $U = V_\perp$ are plotted in Fig. S4. We fit the exponent $2/K$ of the leading term using log-log scale data. The fitted result for $2/K$ decreases from ~ 0.96 to ~ 0.46 as $U = V_\perp$ is increased from 2 to 3.2. From Fig. S4, we also observe subleading oscillations. In our predictions Eq. (S4), these subleading exponents are at least larger than the leading exponent by addition of $K/2$. Using the fitting result of $2/K$, this indicates that the exponent difference $K/2$ ranges from ~ 1.04 to ~ 2.17. Observing nonuniversal exponents numerically, we conclude that the transition line is of Gaussian type.

F. Corrected bosonization of Δ_{D} and Δ_{S}

The two-band bosonization previously reported in the literature has missed the possibility of a terminated transition. In this section, we present a corrected way of doing two-band bosonization of Δ_{D} and Δ_{S}. Recall from

Eq. (5),

$$\Delta_{\mathrm{D}j} = (c_{j,\mathrm{A},\uparrow}c_{j,\mathrm{B},\downarrow} + c_{j,\mathrm{B},\uparrow}c_{j,\mathrm{A},\downarrow})/\sqrt{2},$$
$$\Delta_{\mathrm{S}j} = (c_{j,\mathrm{A},\uparrow}c_{j,\mathrm{A},\downarrow} + c_{j,\mathrm{B},\uparrow}c_{j,\mathrm{B},\downarrow})/\sqrt{2}. \quad \text{(S11)}$$

We note that Δ_{D} and Δ_{S} do not transform with different parity under any symmetry of the Hamiltonian. We aim to reconcile this fact with the fact that using bosonization, these two order parameters appear to give separate quasi-long-range orders in d- and s- paired liquids respectively. (The d-wave and s-wave states are the doped D-Mott and S-Mott respectively.) With the correction, bosonization also concludes that their existence is not mutually exclusive. We will discuss the microscopic definition of s- and d- paired liquids.

We introduce the symbols

$$\psi_{k_y,\eta,\sigma} = \frac{\kappa_{k_y,\sigma}}{\sqrt{2\pi}} e^{i(\theta_{k_y,\sigma}+\eta\phi_{k_y,\sigma})} \quad \text{(S12)}$$

for convenience. Then we can write Eq. (S7) as

$$c_{k_y,\sigma}(x_j) = \sum_{\eta=-1,1} e^{ik_{\mathrm{F},k_y\sigma}x_j}\psi_{k_y,\eta,\sigma} + ..., \quad \text{(S13)}$$

where ... represents neglected higher harmonics.

$$\Delta_{\mathrm{S}} = \sum_{\eta,\eta'=\pm1} [\psi_{0,\eta,\uparrow}\psi_{0,\eta',\downarrow} + \psi_{\pi,\eta,\uparrow}\psi_{\pi,\eta',\downarrow}] + ...,$$
$$\Delta_{\mathrm{D}} = \sum_{\eta,\eta'=\pm1} [\psi_{0,\eta,\uparrow}\psi_{0,\eta',\downarrow} - \psi_{\pi,\eta,\uparrow}\psi_{\pi,\eta',\downarrow}] + ..., \quad \text{(S14)}$$

where higher harmonic terms have been neglected. Using Eq. (S12), we obtain

$$\begin{aligned}
&\sum_{\eta,\eta'=\pm1} \psi_{0,\eta,\uparrow}\psi_{0,\eta',\downarrow} \\
&= C_0 e^{i\sum_\sigma \theta_{0,\sigma}} \cos(\phi_{0,\uparrow} - \phi_{0,\downarrow}) + ... \\
&= C_0 e^{i\sum_\sigma \theta_{0,\sigma}} [\cos(\tilde{\phi}_{+,s})\cos(\tilde{\phi}_{-,s}) - \sin(\tilde{\phi}_{+,s})\sin(\tilde{\phi}_{-,s})] + ... \\
&\sum_{\eta,\eta'=\pm1} \psi_{\pi,\eta,\uparrow}\psi_{\pi,\eta',\downarrow} \\
&= C_\pi e^{i\sum_\sigma \theta_{\pi,\sigma}} \cos(\phi_{\pi,\uparrow} - \phi_{\pi,\downarrow}) + ... \\
&= C_\pi e^{i\sum_\sigma \theta_{\pi,\sigma}} [\cos(\tilde{\phi}_{+,s})\cos(\tilde{\phi}_{-,s}) + \sin(\tilde{\phi}_{+,s})\sin(\tilde{\phi}_{-,s})] + ...
\end{aligned} \quad \text{(S15)}$$

where oscillatory terms and higher harmonics have been neglected; we explicitly write out the coefficients C_0 and C_π, which depend on parameters of Hamiltonian. The subtle issue is that with interaction, one cannot correctly obtain the values of C_0 and C_π by a naive multiplication of vertex operators' coefficients. Unlike the noninteracting limit where $C_0 = C_\pi$ because there is no exchange symmetry of π and 0 bands, we expect $C_0 \neq C_\pi$ for general interacting cases. Using the convention that $\tilde{\phi}_{-,s}$ and $\tilde{\phi}_{-,s}$ are locked at 0 for d- and s- wave paring and for the purpose of evaluating their quasi-long-range orders, Eq. (S11) can be written as

$$\Delta_{\mathrm{S}} \propto e^{i\tilde{\theta}_{+,c}}[C_0\cos(\tilde{\theta}_{-,c}) + (C_\pi - C_0)e^{i\tilde{\theta}_{-,c}}] + ...$$
$$\Delta_{\mathrm{D}} \propto e^{i\tilde{\theta}_{+,c}}[C_0\sin(\tilde{\theta}_{-,c}) - (C_\pi - C_0)e^{i\tilde{\theta}_{-,c}}] + ..., \quad \text{(S16)}$$

In the convention, $\tilde{\theta}_{-,c}$ is locked at 0 and $\pi/2$ for s- and d-pairing states respectively. Thus if $C_0 = C_\pi$, only quasi-long-range order of Δ_{S} exists for s-wave states; the same applies to d-wave. Given that $C_0 \neq C_\pi$ in general, we have both quasi-long-range orders in either s- and d-wave states; in other words, $\langle\Delta_{\mathrm{S}j}\Delta^\dagger_{\mathrm{S},j+d}\rangle$ and $\langle\Delta_{\mathrm{D}j}\Delta^\dagger_{\mathrm{D},j+d}\rangle$ decay algebraically in $|d|$ with the same exponent. However, we can still have a microscopic definition of s-wave and d-wave states. If the leading algebraic decay prefactor of $\langle\Delta_{\mathrm{S}j}\Delta^\dagger_{\mathrm{S},j+d}\rangle$ is larger, we call the state s-wave, otherwise d-wave. This is equivalent to the definition from the relative sign of the coefficient of the leading algebraic decay components of $\langle\Delta_{0,\mathrm{j}}\Delta^\dagger_{0,\mathrm{j+d}}\rangle$ and $\langle\Delta_{\pi,\mathrm{j}}\Delta^\dagger_{\pi,\mathrm{j+d}}\rangle$, where $\Delta_{\mathrm{k_y,j}} = c_{j,k_y,\uparrow}c_{j,k_y,\downarrow}$ A positive relative sign is defined as s-wave states and a negative relative sign is defined as d-wave states. Such a definition no longer necessitates a transition between s- and d-states. A definition via the sign is closely related to our definition of S- and D-Mott using the sign of $\langle O_j\rangle$.

G. Analytical solution for a single rung

In this section, we discuss the analytical solution of a single rung at half filling (which amounts to analyzing a 4×4 matrix) and discuss what one can learn from it for the full model.

The Hamiltonian of the minimal model on a single rung can be written as:

$$\begin{aligned}
H_{\mathrm{rung}} = &-t_\perp \sum_\sigma \left(c^\dagger_{\mathrm{A}\sigma}c_{\mathrm{B}\sigma} + h.c.\right) \\
&+ U\left(n_{\mathrm{A}\uparrow}n_{\mathrm{A}\downarrow} + n_{\mathrm{B}\uparrow}n_{\mathrm{B}\downarrow}\right) \\
&+ V_\perp \sum_{\sigma\sigma'} n_{\mathrm{A}\sigma}n_{\mathrm{B}\sigma'} + V_\perp - V_\perp \sum_\sigma \left(n_{\mathrm{A}\sigma} + n_{\mathrm{B}\sigma}\right).
\end{aligned} \quad \text{(S17)}$$

At half filling we can replace $\sum_\sigma (n_{\mathrm{A}\sigma} + n_{\mathrm{B}\sigma}) = 2$ and use the basis states $c^\dagger_{\mathrm{A}\uparrow}c^\dagger_{\mathrm{B}\downarrow}|\Omega\rangle = |\uparrow,\downarrow\rangle$, $c^\dagger_{\mathrm{A}\downarrow}c^\dagger_{\mathrm{B}\uparrow}|\Omega\rangle = |\downarrow,\uparrow\rangle$, $c^\dagger_{\mathrm{A}\uparrow}c^\dagger_{\mathrm{A}\downarrow}|\Omega\rangle = |\uparrow\downarrow,0\rangle$, $c^\dagger_{\mathrm{B}\downarrow}c^\dagger_{\mathrm{B}\uparrow}|\Omega\rangle = |0,\uparrow\downarrow\rangle$, whereby $|\Omega\rangle$ is the vacuum. In this basis, the Hamiltonian matrix reads:

$$H = \begin{pmatrix} 0 & 0 & -t_\perp & -t_\perp \\ 0 & 0 & +t_\perp & +t_\perp \\ -t_\perp & +t_\perp & U - V_\perp & 0 \\ -t_\perp & +t_\perp & 0 & U - V_\perp \end{pmatrix}. \quad \text{(S18)}$$

This is a two-site Hubbard problem, extended by $V_\perp$. We see that for a single rung, its effect is to simply shift $U \to U - V_\perp$ (which is not generally true for the full

ladder). The eigenstates can be characterized by the spin and pseudospin quantum numbers (which we call "S" and "T", respectively), whereby the pseudospin operators for a bipartite lattice are in general defined as:

$$\begin{aligned} T_i^- &= (-1)^i c_{i\downarrow} c_{i\uparrow}, \\ T_i^+ &= (-1)^i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger, \\ T_i^z &= \frac{1}{2}\left(n_i - 1\right), \end{aligned} \tag{S19}$$

and fulfill SU(2) algebra relations $\left[T_i^z, T_j^\pm\right] = \pm\delta_{ij} T_i^\pm$, $\left[T_i^+, T_j^-\right] = 2\delta_{ij} T_i^z$. For a single rung the indices are $i, j = \mathrm{A}, \mathrm{B}$.

Two of the four eigenstates are the spin-triplet and the pseudospin-triplet:

- spin-triplet:
  $\left|S=1, M_S=0\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow,\downarrow\right\rangle + \left|\downarrow,\uparrow\right\rangle\right)$
  $E = 0$
- pseudospin-triplet:
  $\left|T=1, M_T=0\right\rangle = \frac{1}{\sqrt{2}}\left(\left|0,\uparrow\downarrow\right\rangle - \left|\uparrow\downarrow,0\right\rangle\right)$
  $E = U - V_\perp$

The corresponding singlets are:

- spin-singlet:
  $\left|S=0\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow,\downarrow\right\rangle - \left|\downarrow,\uparrow\right\rangle\right)$
- pseudospin-singlet:
  $\left|T=0\right\rangle = \frac{1}{\sqrt{2}}\left(\left|0,\uparrow\downarrow\right\rangle + \left|\uparrow\downarrow,0\right\rangle\right)$

However, they are not by themselves eigenstates. Instead, one needs to form a "bonding" and and an "antibonding" superposition:

- bonding singlet superposition:
  $\left|S=T=0,-\right\rangle = \alpha_- \left|S=0\right\rangle + \beta_- \left|T=0\right\rangle$
  $E_- = \frac{U-V_\perp}{2} - \sqrt{\left(\frac{U-V_\perp}{2}\right)^2 + 4t_\perp^2}$
- antibonding singlet superposition:
  $\left|S=T=0,+\right\rangle = \alpha_+ \left|S=0\right\rangle + \beta_+ \left|T=0\right\rangle$
  $E_+ = \frac{U-V_\perp}{2} + \sqrt{\left(\frac{U-V_\perp}{2}\right)^2 + 4t_\perp^2}$

The mixing coefficients are given by:

$$\begin{aligned} \alpha_\pm &= \frac{1}{\sqrt{1 + E_\pm^2/(4t_\perp^2)}}, \\ \beta_\pm &= -\frac{E_\pm}{2t_\perp}\frac{1}{\sqrt{1 + E_\pm^2/(4t_\perp^2)}}. \end{aligned} \tag{S20}$$

The bonding singlet superposition is always the ground state. It contains more spin-singlets in the admixture for $U > V_\perp$ (which becomes the D-Mott phase on the ladder), more "pseudo-singlets" (on-site singlets) for $U < V_\perp$ (which becomes the S-Mott phase); and an equal superposition $\frac{1}{\sqrt{2}}\left(\left|S=0\right\rangle + \left|T=0\right\rangle\right)$ for $U = V_\perp$, which we call a "rung bisinglet" in the main text.

In the strong-coupling limit $\left|U - V_\perp\right| \gg t_\perp$ and for $U > V_\perp$, we have $E_- \approx -4\frac{t_\perp^2}{U-V_\perp} = J$, and the two low-lying states become the spin-singlet and spin-triplet, split in energy by J, indicating an effective Heisenberg model.

On the other hand, if $V_\perp < U$, we obtain $E_- \approx U - V_\perp + J$ and the two low-lying states become the pseudospin singlet and pseudospin triplet, again split in energy by J. We see that even though the density-density interaction of the original model is of Ising type and only couples the z-components of the pseudospin, the strong-coupling limit favors entangled singlet states. This is because we have restricted ourselves to half filling for the rung, where $V_\perp$ acts exactly as an attractive $U < 0$.

For the full ladder, both $V_\perp > 0$ and $U < 0$ favor an S-Mott phase, but the effect of $V_\perp$ cannot be simply captured by substituting $U \to U - V_\perp$. Doing so neglects charge fluctuations on the rungs and will not reveal the terminated transition.

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