Two-Fluid Coexistence in a Spinless Fermions Chain with Pair Hopping

Lorenzo Gotta,[1,*] Leonardo Mazza,[1] Pascal Simon,[2] and Guillaume Roux[1]
[1]*Université Paris–Saclay, CNRS, LPTMS, 91405 Orsay, France*
[2]*Université Paris–Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France*

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We show that a simple one-dimensional model of spinless fermions with pair hopping displays a phase in which a Luttinger liquid of paired fermions coexists with a Luttinger liquid of unpaired fermions. Our results are based on extensive numerical density-matrix renormalization-group calculations and are supported by a two-fluid model that captures the essence of the coexistence region.

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The search for zero-energy Majorana modes, which naturally appear in topological superconducting models [1], has raised remarkable interest in the problem of pairing in number-conserving models [2–16]. A paired phase is a phase where two (or more) fermions bind together and behave as a singular molecular object. In one dimension, where most attention has concentrated thus far, the characteristic signature of pairing is the absence of any fermionic order, whereas pairs display quasi-long-range order. For spin-$1/2$ fermions, the attractive Hubbard model naturally favors on-site singlet pairing [17,18]. Increasing the number of internal degrees of freedom allows a pairing mode to coexist with a remaining decoupled fermionic mode [19]. For spinless fermions, pairing requires finite-range interaction but no coexistence with unpaired fermions is observed [20–23]. Importantly, spatial interfaces between paired and unpaired phases should host Majorana zero modes, which could then be realized without resorting to superconducting proximity effects [24,25].

The difficulty in studying the pairing transition is that it implies a reshaping of the low-energy sector of the model, with the appearance (or disappearance) of Fermi points, to be taken into account by unconventional bosonization treatments [24,25]. A particularly visual model based on two fluids, a bosonic one describing the pairs and a fermionic one describing the unpaired fermions, was presented recently [26]. These studies agree on the fact that paired and unpaired phases are separated by a continuous phase transition with central charge $c = 3/2$ [24,26] originating from a standard gapless mode and an additional Ising or Majorana degree of freedom. This prediction has been verified in several numerical analyses [20–23].

In this Letter, we show that the phenomenology of the pairing transition is richer. We revisit a one-dimensional (1D) spinless-fermion model introduced in Ref. [25] in which pair hopping competes with single-fermion hopping. Related electronic models with correlated hopping, such as the Penson-Kolb-Hubbard model [27–32], have been proposed in the context of high-T_c superconductors [33] and lead to rich and complex phase diagrams [34]; our model also bears some relationship with the folded spin-$1/2$ model [35,36] and the Bariev model, which are exactly solvable with the Bethe ansatz [37], and with models for ultracold gases with synthetic dimension [38,39].

We show the emergence of a coexistence phase comprising neighboring paired fermions in a sea of unpaired fermions that is stable toward phase separation. Since pairs are composed of two fermions, it is not obvious that they could coexist with gapless fermionic excitations. Indeed, semiclassical intuition and the standard Luttinger liquid (LL) approach lead to the conclusion that all fermions are either paired or unpaired. Yet, taking superfluids as a paradigmatic example, phases with two coexisting fluids are not novel to condensed-matter physics [40]. Our findings are supported by numerical simulations, which are fully interpreted with a phenomenological two-fluid (2F) model inspired by Ref. [26]. In particular, we clearly pinpoint under which conditions the two kinds of scenarios, the extended coexistence phase and a $c = 3/2$ transition point, take place (see also Ref. [41]). Such a discovery of the first realization of a 2F model for describing a 1D phase with a pairing instability opens the path to novel investigations in the context of number-conserving Majorana fermions.

Hamiltonian.—We consider a chain of length L with spinless fermion operators $c_j^{(\dagger)}$ and study the model introduced in Ref. [25],

$$H = -t\sum_j [c_j^\dagger c_{j+1} + \mathrm{H.c.}] - t'\sum_j [c_{j+1}^\dagger c_j^\dagger c_j c_{j-1} + \mathrm{H.c.}], \tag{1}$$

in which t is the fermionic hopping amplitude while t' is the pair-hopping amplitude. The phase diagram depends only on the ratio $\tau = t'/t$ and the density $n = N/L$, with N the total number of fermions. The unusual t' term favors a gain

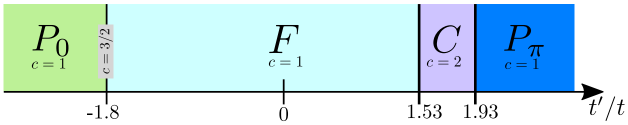

FIG. 1. Sketch of the phase diagram of model (1) for density $n = 0.25$. Four phases appear: a regular LL fermionic phase F, paired LL phases P_0 and P_π, and a coexistence phase C with central charge $c = 2$ where fermions and P_π pairs are mixed.

in kinetic energy for paired configurations that naturally competes at low densities with the single-fermion kinetic energy term (a similar term has been identified in cold-atom setups with synthetic dimensions [38,39]). We take $n = 0.25$ in the following and analyze such competition with the density-matrix renormalization-group (DMRG) algorithm [42–45] using two implementations, one of which is the ITensor library [46], both working with a fixed number of particles. The obtained phase diagram is sketched in Fig. 1. For small τ a regular fermionic LL phase F extends from the free fermion point. At large $|\tau|$, two fully paired LL phases P_0 and P_π are stabilized. Their main difference is that pairs quasicondense around either the $k = 0$ or the $k = \pi$ momenta. All three phases display a central charge $c = 1$ corresponding to a single bosonic mode description. For $\tau < 0$, it has been shown [25] that the transition from F to P_0 is direct and features an extra Majorana degree of freedom revealed from the $c = 3/2$ central charge. The main result of this Letter is to show that for $\tau > 0$, there is an intervening coexistence phase denoted by C where a LL of P_π pairs coexists with a LL of fermions.

Paired phases.—We first analyze the paired phases exploiting the fact that model (1) can be diagonalized exactly [35,39] for $t = 0$. Since the pair-hopping term enhances the kinetic energy of pairs, we assume that the ground state lies in the subspace $\mathcal{H}_P$ spanned by states with the $2N_b$ fermions forming N_b nearest-neighbor pairs. Within $\mathcal{H}_P$, each fermionic state is mapped onto a spin-1/2 configuration over a lattice of length $L_b = L - N_b$ via the rules $|\bullet\bullet\rangle \to |\uparrow\rangle$, $|\circ\rangle \to |\downarrow\rangle$. In L_b, the N_b term can be understood as an excluded volume. Then, a spin up stands for a pair while a spin down stands for an empty site. The action of Hamiltonian (1) over $\mathcal{H}_P$ is equivalent to that of an effective XX spin-1/2 Hamiltonian $H_{\text{eff}} = t' \sum_{j=1}^{L_b} [\sigma_j^+ \sigma_{j+1}^- + \text{H.c.}]$. Using the Jordan-Wigner transformation and the Fourier transform, we readily find the diagonal form $H_{\text{eff}} = \sum_k \varepsilon_p(k) n_k$, with the pair band dispersion relation $\varepsilon_p(k) = 2t' \cos(k)$. For $t' < 0$, the ground state energy per site $e_{\text{eff}} = \langle H_{\text{eff}} \rangle / L$ reads

$$e_{\text{eff}} = \frac{1}{L} \sum_{|k| < \pi(N_b/L_b)} \varepsilon_p(k) = -\frac{2|t'|}{\pi} \left(1 - \frac{n}{2}\right) \sin\left(\frac{\pi n}{2 - n}\right), \tag{2}$$

where we use the relation $n = 2N_b/L$. For $t' > 0$, one actually has the same result because the unitary transformation

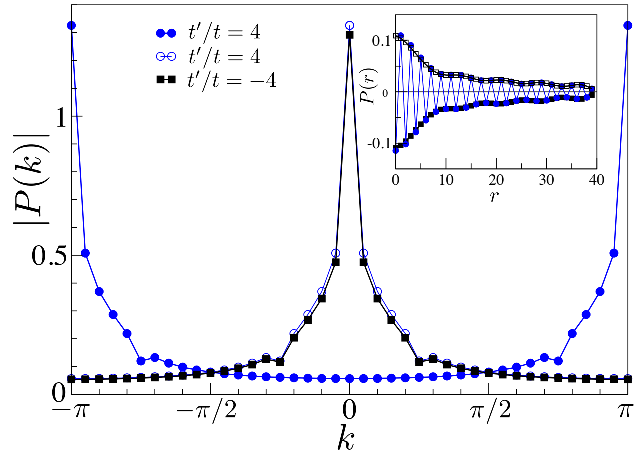

FIG. 2. Absolute value of the Fourier transform of pair correlations for an open chain with $L = 80$ and $t'/t = \pm 4$. Open symbols are the $t'/t = 4$ data shifted by π. Inset: pair correlations.

$c_j \to e^{i(\pi/2)j} c_j$ implements the mapping $H(t = 0, t') \to H(t = 0, -t')$. Equation (2) is validated by the numerics [47].

The nature of the pairs is qualitatively different in each phase. By inspecting $\varepsilon_p(k)$, we see that the minimum is at $k = \pi$ for $t' > 0$, whereas it lies at $k = 0$ for $t' < 0$. The two phases are thus connected by a shift $k \to k + \pi$, corresponding to the application of the unitary transformation to the pair operator: $c_j c_{j+1} \to (-1)^j i c_j c_{j+1}$. This difference persists at finite but large $|\tau|$. In the inset of Fig. 2, we show the pair correlations $P(r) = \langle c_{L/2}^\dagger c_{L/2+1}^\dagger c_{L/2+r} c_{L/2+r+1} \rangle$ for $\tau = \pm 4$. They almost exactly coincide in absolute value but differ by a staggering factor $(-1)^r$. The main chart of Fig. 2 displays the pair occupation number $P(k) = (1/L) \sum_{j,j'} e^{ik(j-j')} \langle c_j^\dagger c_{j+1}^\dagger c_{j'} c_{j'+1} \rangle$. The connection between P_π and P_0 translates into a shift of the main peak from $k = \pi$ to $k = 0$ when changing $\tau = 4$ into $\tau = -4$. Notice that the unitary transformation is no longer valid at nonzero t at the Hamiltonian level. Still, the data show that it becomes an emergent symmetry due to the dominant weights of paired states. Since the transition between the fermionic LL and P_0 phases was extensively discussed in Ref. [25], we now focus on $\tau > 0$ [48].

Coexistence phase.—We now present numerical results for the intervening coexistence phase C between the F and P_π LL. In Figs. 3(a) and 3 (a′), we plot the first and second derivatives of the ground state energy per site $e_0(\tau)$. While constant behaviors are found in F and P_π, a finite intermediate region emerges between two finite jumps of the second derivative. Since the first derivative is continuous up to finite-size effects, we observe two continuous phase transitions that mark the existence of the C phase, in contrast to the first-order transition scenario proposed in Ref. [25] and as will be clear in the following. Within the grid precision, the boundaries of this C phase are found at $\tau_{c1} \simeq 1.53(1)$ and $\tau_{c2} \simeq 1.93(1)$. Last, increasing the system sizes shows that the phase is stable and does not shrink, as can be seen in the figure.

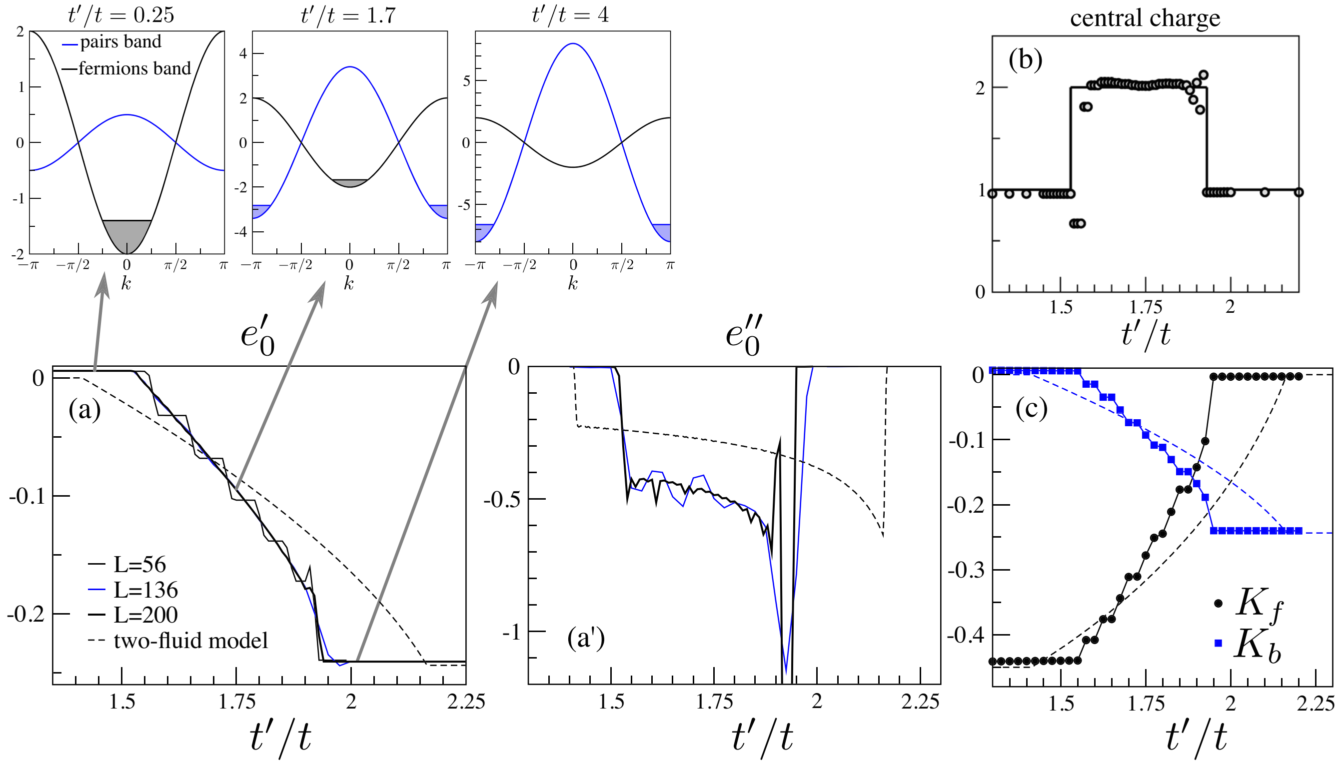

FIG. 3. (a) First and (a′) second derivatives of the energy per site e_0 as a function of t'/t for three system sizes: $L = 56$, 136, 200. Dotted lines are predictions of the 2F model. Arrows point toward typical band structures of the 2F model for $t'/t = 0.25$, $t'/t = 1.7$, and $t'/t = 4$. (b) Fitted central charges as a function of t'/t. (c) Single-particle kinetic energy K_f and pair kinetic energy K_b probing almost directly n_f and n_b.

A first insight in the nature of the C phase is presented in Fig. 3(b). We show that the central charge c, estimated from fits of the entanglement entropy [47], jumps from $c = 1$ in F and P_π to the value $c = 2$ in the C phase. These values indicate that the F and P_π phases have a single effective bosonic mode, whereas the C phase possesses two bosonic modes that will be identified in the following. In the rest of the Letter, we develop an effective model that (i) captures the low-energy physics of the Hamiltonian (1), (ii) explains the nature of the C phase, and (iii) elucidates the difference in stability against effective interactions in the $\tau < 0$ and $\tau > 0$ branches of the phase diagram.

Two-fluid model.—We start by assuming that the system is composed of two species of particles, one fermionic (the unpaired fermions) and one bosonic (the pairs), described respectively by a free fermion Hamiltonian H_f and an XX model H_b:

$$H_f = -t\sum_j d_j^\dagger d_{j+1} + \text{H.c.}, \tag{3}$$

$$H_b = +t'\sum_j \sigma_j^+ \sigma_{j+1}^- + \text{H.c.} \tag{4}$$

It is important to stress that this is an effective model and that the d_j fermions (satisfying canonical anticommutation relations) do not coincide with the original ones, because they describe only the unpaired particles. This assumption is motivated by the limiting properties of the Hamiltonian (1) for $t = 0$ and $t' = 0$ that we discussed above. We stress, however, that there is no exact handy mapping onto Eq. (1): the 2F model $H_{2F} = H_f + H_b$ has a phenomenological nature.

As a minimal model, we further assume that the two species interact only through the total density constraint $n = n_f + 2n_b$, where $n_{f,b} = N_{f,b}/L$ are the effective fermionic and bosonic densities. The ground state energy per site e_{2F} is then the sum of the fermionic and bosonic contributions:

$$e_{2F} = -\frac{2t}{\pi}\left[\sin(\pi n_f) + \tau \sin\left(\pi\frac{n - n_f}{2}\right)\right]. \tag{5}$$

By minimizing e_{2F} with respect to the free parameter n_f using standard techniques [47], we identify three regions that are depicted in the sketches of Fig. 3: (i) a fully fermionic region, for $0 < \tau < \tau_{c1}$ with $\tau_{c1} = 2\cos(\pi n) \simeq 1.41$, in which $n_f = n$ and $n_b = 0$, that we associate to the F phase; (ii) an intermediate region, for $\tau_{c1} < \tau < \tau_{c2}$ with $\tau_{c2} = 2/\cos(\pi n/2) \simeq 2.16$, in which both n_f and n_b are nonzero, that we associate with the C phase; and (iii) a fully bosonic region, for $\tau > \tau_{c2}$, in which $n_f = 0$ while

$n_b = n/2$, corresponding to the P_π phase. Incidently, the natural order parameter through the phase diagram is n_f (or, equivalently, n_b). In this two-fluid picture, (ii) is naturally a region of *coexistence* of the bosonic and fermionic fluids; hence the name.

The 2F model thus proposes an interpretation of the two transition points in terms of two band-filling (band-emptying) Lifshitz transitions, which are associated with the appearance (disappearance) of two Fermi points, as sketched in Fig. 3(a). We are thus in front of two continuous and second-order quantum phase transitions, and not of a first-order transition, which is another scenario that would be *a priori* possible. In the following, we show that the two-fluid model provides a good description of the C phase.

Interpretation of numerical data.—We first observe that the 2F model describes in a natural way the DMRG data of Fig. 3. The main difference is that the boundary points are not quantitatively reproduced. Let us start with the central charge: in the 2F model, the coexistence phase has $c = 2$, which corresponds to two effective low-energy bosonic fields in LL theory. These modes stem from the effective existence of two gapless Fermi points k_f, leading to a single bosonic mode in LL theory, and two "hard-core boson" Fermi points k_b adding up to another bosonic mode. On the contrary, the F and P_π region have only two effective Fermi points, leading to standard $c = 1$ phases. This agrees perfectly with the numerical data in Fig. 3(b).

We now focus on the comparison with local observables to further characterize the C phase. Focusing on the energy, we superimpose the 2F model prediction for the first and second derivatives $e'_{2\mathrm{F}}(\tau)$ and $e''_{2\mathrm{F}}(\tau)$ to the DMRG data in Figs. 3(a) and 3(a′). We observe two jump discontinuities that are computed exactly in the 2F model [47]. The qualitative resemblance with the numerical data is impressive given the simplicity and phenomenological nature of the 2F model. Furthermore, this total energy splits into two contributions that are directly connected to the order parameters n_f and n_b. We define the single-particle kinetic energy $K_f = -(1/L)\sum_j \langle c_j^\dagger c_{j+1} + \mathrm{H.c.}\rangle$ and the pair-hopping kinetic energy $K_b = -(1/L)\sum_j \langle c_{j+1}^\dagger c_j^\dagger c_j c_{j-1} + \mathrm{H.c.}\rangle$ such that $e_0 = tK_f + t'K_b$ and $K_b = e'_0(\tau)$ according to the Feynman-Hellmann theorem. The 2F model prediction then simply corresponds to each term of Eq. (5). The comparison with DMRG data is displayed in Fig. 3(c) with dotted lines. K_f and K_b capture the order parameter value essentially up to a sine function. We do observe that they are very close to zero in the P_π and F phases, respectively. In the C phase, they both vary following the qualitative behavior obtained within the 2F model. Last, the band-filling interpretation helps one to understand finite-size effects: in both Figs. 3(a) and Fig. 3(c), jumping from one plateau to the next corresponds to filling the system with another pair. For instance, with $L = 56$ there are between 0 and 7 pairs that are progressively created as t' increases.

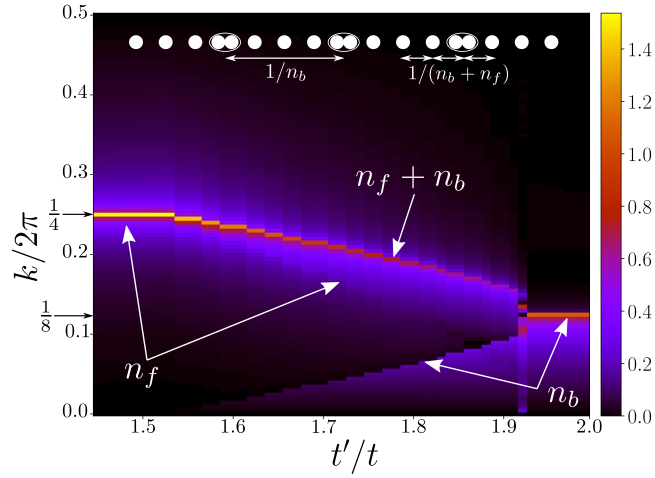

FIG. 4. Map of the absolute value of the Fourier transform of local density fluctuations $\langle \delta n_j \rangle$ as a function of t'/t for an open chain with $L = 200$.

This pair creation is also plainly seen in the density profile obtained with open boundary conditions with DMRG, which fully supports our interpretation of the C phase. We show in Fig. 4 the Fourier transform of the local density fluctuations $\langle \delta n_j \rangle = \langle c_j^\dagger c_j \rangle - n$. Indeed, for the F and P_π, we expect leading fluctuations at $2k_f = 2\pi n$ and $2k_b = \pi n$, respectively. Such constant behaviors are clearly observed in Fig. 4 around the coexistence region by recalling that $n = 0.25$. Within the C phase, the leading fluctuations emerge at $k = 2\pi(n_f + n_b)$, with a second main peak at $k = 2\pi n_b$ and a very small signal at $k = 2\pi n_f$. This is understood from the sketch of Fig. 4. In the C phase, pairs effectively repel each other and add some excluded volume to the remaining unpaired fermions. Then, if one equally spaces the total number $N_f + N_b$ of effective particles, this corresponds to a mean distance of $1/(n_f + n_b)$. On top of that, pairs add an extra signal—since that locally doubles the density—corresponding to a typical spacing of $1/n_b$. Consequently, following the location of the peaks allows one to quantitatively follow the order parameters. Notice that such excluded volume effects go beyond the 2F model picture according to which the fluctuations of the two fluids should be independent.

Phase stability.—If we consider that interactions between fermions and bosons have been totally neglected, the effectiveness of the 2F model looks rather surprising. In reality, as we have seen, these degrees of freedom delocalize in the same 1D setup and effectively repel each other because one site cannot be occupied by one fermion and one boson at the same time. The main consequence of this is that single-particle hopping can create one pair by putting two unpaired fermions close by (and vice versa). At the first level of approximation, we need to include a term like $-t\sum_j(\sigma_j^+ d_j d_{j+1} + \mathrm{H.c.})$. Yet one such term is completely irrelevant because it conserves momentum: the annihilation of two fermions with momentum k_1 and k_2 leads to the creation of one boson with momentum $k_1 + k_2 + 2\pi m$, where $m \in \mathbb{Z}$. As we discussed initially, the fermionic particles are concentrated around $k \sim 0$, whereas the bosonic ones are located around $k \sim \pi$. This term is thus ineffective: it fails to hybridize bosonic and fermionic degrees of freedom and can be safely neglected. On the contrary, the bosons quasicondense around $k = 0$ in between the F and P_0 phases. Interactions are then resonant and hybridize fermionic and bosonic degrees of freedom. According to the description developed in Ref. [26], one then expects a direct continuous transition with central charge $c = 3/2$, which is in agreement with the numerics for $t' < 0$ [25].

Conclusions.—We have presented a study of the pairing transition in a model featuring a competition between the delocalization of fermions and that of pairs. The DMRG results and their interpretation using a simple phenomenological model strongly support the existence of an unexpected coexistence phase of paired and unpaired fermions. These remarkable outcomes put on a more solid basis the 2F model presented in Ref. [26] and provide an open route to wider applications in the context of one-dimensional models featuring paired phases.

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*lorenzo.gotta@universite-paris-saclay.fr

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[47] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.126.206805 for detailed calculations and additional numerical analysis.
[48] We noticed that the numerical data of Ref. [25] actually correspond to the $\tau = t'/t < 0$ case.