Topological Lifshitz transitions, orbital currents, and interactions in low-dimensional Fermi gases in synthetic gauge fields

Chen-How Huang, Masaki Tezuka and Miguel A Cazalilla

1 Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 4, San Sebastian 20018, Spain
2 Department of Physics, Kitashirakawa, Kyoto University, Kyoto 606-8502, Japan
3 IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao, Spain

* Author to whom any correspondence should be addressed.
E-mail: miguel.cazalilla@dipc.org

Keywords: fermions in optical lattices, synthetic gauge fields, orbital currents, strongly correlated fermions, Tomonaga–Luttinger liquids, mean-field theories, Lifshitz quantum phase transitions

Abstract
Low-dimensional systems of interacting fermions in a synthetic gauge field have been experimentally realized using two-component ultra-cold Fermi gases in optical lattices. Using a two-leg ladder model that is relevant to these experiments, we have studied the signatures of topological Lifshitz transitions and the effects of the inter-species interaction $U$ on the gauge-invariant orbital current in the regime of large intra-leg hopping $\Omega$. Focusing on non-insulating regimes, we have carried out numerically exact density-matrix renormalization-group (DMRG) calculations to compute the orbital current at fixed particle number as a function of the interaction strength and the synthetic gauge flux per plaquette. Signatures of topological Lifshitz transitions where the number Fermi points changes are found to persist even in the presence of very strong repulsive interactions. This numerical observation suggests that the orbital current can be computed from an appropriately renormalized mean-field band structure, which is also described here. Quantitative agreement between the mean-field and the DMRG results in the intermediate interaction regime where $U \lesssim \Omega$ is demonstrated. We also have observed that interactions can change the sign of the current susceptibility at zero field and induce Lifshitz transitions between two metallic phases, which is also captured by the mean-field theory. Correlation effects beyond mean-field theory in the oscillations of the local inter-leg current are also reported. We argue that the observed robustness against interactions makes the orbital current a good indicator of the topological Lifshitz transitions.

1. Introduction
Ultracold gases in artificial gauge fields have opened the possibility of quantum simulating condensed matter systems subject to strong (orbital) magnetic or spin–orbit fields [1–8]. In recent experiments [8–13], it has been possible to simulate fermionic multi-leg ladders subject to a strong (orbital) magnetic field using a Raman laser to couple different internal degrees of freedom (corresponding to different orientations of the nuclear spin of alkaline-earth-like atoms (AEA)). Thus, the strong inter-leg hopping limit can be achieved by direct control of the Raman lasers. Besides, the Raman lasers provide the atoms a finite momentum kick, which simulates an abelian gauge field. An AEA can be regarded as a spin-$F$ particle where $F$ stands for the nuclear spin. Its $2F+1$ spin states can be coupled by laser-induced complex hopping, leading to a $2F+1$ leg ladders of neutral atoms in a synthetic gauge field [8–14]. This situation approaches the 2D system limit for large $F$. Experimentally, several groups have been using synthetic gauge fields in attempts to emulate multi-leg systems in magnetic fields that may display topological ordered
We shall consider a fermionic two-leg ladder system described by the following Hamiltonian:

\[ H = H_{\parallel} + H_{\perp} + H_U, \]  
\[ H_{\parallel} = -t \sum_{m,\sigma} \left[ \tilde{c}_{m,\sigma}^\dagger \tilde{c}_{m+1,\sigma} + h.c. \right], \]  
\[ H_{\perp} = \tilde{c}_{m,\sigma} \tilde{c}_{m,\sigma}^\dagger + \text{h.c.}, \]  
\[ H_U = \sum_{m,\sigma} \sigma \tilde{c}_{m,\sigma} \tilde{c}_{m,\sigma}^\dagger, \]  

2. Model and gauge invariance

We shall consider a fermionic two-leg ladder system described by the following Hamiltonian:

\[ H = H_{\parallel} + H_{\perp} + H_U, \]  
\[ H_{\parallel} = -t \sum_{m,\sigma} \left[ \tilde{c}_{m,\sigma}^\dagger \tilde{c}_{m+1,\sigma} + h.c. \right], \]  
\[ H_{\perp} = \tilde{c}_{m,\sigma} \tilde{c}_{m,\sigma}^\dagger + \text{h.c.}, \]  
\[ H_U = \sum_{m,\sigma} \sigma \tilde{c}_{m,\sigma} \tilde{c}_{m,\sigma}^\dagger, \]  

phases such as (fractional) quantum Hall states [3–7, 15, 16], and exhibit gapless chiral edge modes [9–11, 17–19].

However, to the best of our knowledge, fewer studies have focused on the experimentally realized strong inter-leg hopping limit and experimentally accessible gauge-invariant observables such as the orbital current. Unlike transport [16, 20] or (non-quantized) Hall currents [21] in response to an electric field, the orbital current is a ground state property and does not depend on the non-equilibrium distribution of the low-lying degrees of freedom [22, 23]. Therefore, in order to understand the effects of interaction on it, it cannot be computed using field-theory methods like e.g. bosonization [20]. Indeed, the orbital current contains information about the entire band structure and not just the degrees of freedom close to the Fermi energy [22, 23]. Furthermore, as we show here, at least in a certain parameter range, the interaction effects can be accounted for by mean-field theory. This approach reveals valuable information about the effects of interaction and its interplay with the (synthetic) gauge field. We have benchmarked the mean-field theory against density-matrix renormalization group (DMRG) [24–27] calculations of the orbital current. In the limit of large inter-leg hopping and moderate interaction the mean-field theory can describe the effect of inter-leg interactions. Qualitatively, this is because the inter-leg interaction leads to an effective enhancement of the inter-leg hopping since interactions favor the same type of ground state configurations as the inter-leg hopping.

As described below, the orbital current displays cusps at certain values of the flux per plaquette or the interaction. In the non-interacting limit, such cusps are related to topological Lifshitz (quantum phase) transitions where the topological properties of the Fermi surface change. In one dimension, the number of disconnected components of the Fermi 'surface', i.e. number of Fermi points, changes. Mathematically, this is described by a change in the zeroth order homotopy group, \( \pi_0 \). By using DMRG to compute the orbital current, we have found that such cusps are robust in presence of strong interactions. The mean-field theory described below is also able to quantitatively describe such cusps for weak to moderate repulsive interactions. This suggests that it is possible to interpret the Lifshitz transitions as transitions of a renormalized (mean-field) band structure.

Topological Lifshitz transitions have attracted much attention in a variety strongly correlated materials such as heavy fermions [28], pnictide superconductors [29], and more recently twisted bilayer graphene [30]. In a recent years, Volovik [31] has emphasized the importance of Lifshitz transitions in interacting systems and the non-trivial interplay of topology and interactions, in particular in connection to flat band formation. In this context, the study reported in this article concerns the effect of Lifshitz transitions in a one-dimensional system for which interactions are known to have very dramatic effects on the single-particle excitations [20]. In contrast, our findings support the applicability of mean-field theory to describe interaction effects on the orbital current. In addition, the mean field theory predicts the existence of interaction-driven Lifshitz transitions, which is confirmed by our DMRG calculations.

Due to their large tunability, ultra-cold atomic systems appear to be an ideal platform to address some of the deep questions posed by the interplay of interactions and topological Lifshitz transitions. Indeed, experimental and theoretical work along this direction has been reported in reference [32]. This study reported the experimental observation of a Lifshitz transition for a trapped Fermi gas subject to an artificial spin–orbit coupling. However, unlike the one-dimensional Fermi gases studied here, this system is not a strongly correlated one, and therefore it is not surprising that mean-field theory can be applied. In addition, no study of the behavior of the orbital current across the Lifshitz transition was reported in reference [32].

The following sections are organized as follows: in section 2, we introduce the model and discuss how the orbital current can be measured in the ultracold atom setup together with the issue of gauge invariance of observables. In section 4, we discuss the effect of inter-leg interaction using DMRG. The DMRG results are compared to perturbation theory and mean-field theory. We also discuss the mean-field theory prediction of an interaction-induced Lifshitz transition, which is confirmed using DMRG to compute the orbital and inter-leg currents. Finally, we provide a summary and discussion of the results together with an outlook of our work in section 5. We have relegated to the appendices some of most technical details of the calculations as well as the review of some important results for non-interacting systems.

2. Model and gauge invariance

We shall consider a fermionic two-leg ladder system described by the following Hamiltonian:

\[ H = H_{\parallel} + H_{\perp} + H_U, \]  
\[ H_{\parallel} = -t \sum_{m,\sigma} \left[ \tilde{c}_{m,\sigma}^\dagger \tilde{c}_{m+1,\sigma} + h.c. \right], \]  
\[ H_{\perp} = \tilde{c}_{m,\sigma} \tilde{c}_{m,\sigma}^\dagger + \text{h.c.}, \]  
\[ H_U = \sum_{m,\sigma} \sigma \tilde{c}_{m,\sigma} \tilde{c}_{m,\sigma}^\dagger, \]
New J. Phys. 24 (2022) 033043
C-H Huang et al

\[ H_\perp = -\frac{\Omega}{2} \sum_m \left[ e^{-i\phi_m} \tilde{c}_m^\dagger \tilde{c}_{m+1} + \text{h.c.} \right] , \]  
\[ H_U = U \sum_m \tilde{n}_{m,\uparrow} \tilde{n}_{m,\downarrow} . \]  

In the above expression \( t (\Omega) \) is the intra-leg (inter-leg) hopping, and \( \tilde{n}_{m,\sigma} = \tilde{c}_m^\dagger \tilde{c}_m \). The operators \( \tilde{c}_m \) and \( \tilde{c}_m^\dagger \) obey \( \{ \tilde{c}_m, \tilde{c}_m^\dagger \} = \delta_{m,m'} \), anti-commuting otherwise. Anticipating that in ultracold atomic systems the legs of the ladder may correspond to different internal degrees of freedom or to the excited and ground states of the same atom species [9], we use a pseudo-spin index \( \sigma = \uparrow, \downarrow \) to denote the chain index. In this notation, the orbital current can also be regarded as a pseudo-spin current (cf equation (19)). An interaction of the Hubbard type acts on atoms with different pseudo-spin or leg index \( \sigma \). Concerning this feature, we recall that, at ultracold temperatures, interactions are well described by a short-range pseudo-potential which leads to equation (4) when projected on the Wannier orbitals of the lowest Bloch bands. In the above expression, \( \phi \) corresponds to the flux of the Aharonov–Bohm phase of pseudo-gauge field accumulated by an atom when going around a plaquette (see figure 1). Finally, note that in equation (1) and in all the equations below, we work in units where the lattice constant \( a = 1 \) and the reduced Planck’s constant \( \hbar = 1 \).

Let us perform a (unitary) gauge transformation such that

\[ \epsilon_{m,\sigma} = \tilde{c}_{m,\sigma} e^{i\phi_m} . \]  

By introducing \( \phi_\uparrow \) and \( \phi_\downarrow \) obeying \( \phi_\uparrow - \phi_\downarrow = \phi \), the site dependence in the phase of the inter-leg hopping term, \( H_\perp \), can be removed at the cost of introducing (position-independence) phases in the intra-leg hopping terms of the Hamiltonian, i.e.

\[ H_{\perp,1} = -i \sum_{m,\sigma} \left[ e^{i\phi} \epsilon_{m,\sigma}^\dagger \epsilon_{m+1,\sigma} + \text{h.c.} \right] \]  
\[ H_{\perp,2} = -\Omega \sum_m \left[ \epsilon_m^\dagger \epsilon_m + \text{h.c.} \right] . \]  

Note that the gauge transformation (5) does not affect the site occupation operators, i.e.

\[ n_{m,\sigma} = \tilde{c}_{m,\sigma}^\dagger \tilde{c}_{m,\sigma} = \tilde{c}_{m,\sigma}^\dagger \tilde{c}_{m,\sigma} = \tilde{n}_{m,\sigma}, \]  
and therefore the form of the interaction is not altered. Let us recall that, in condensed matter systems, all observables are gauge invariant and do not depend on the particular choice of the phases \( \phi_\sigma \). On the other hand, in ultracold atomic systems, non-gauge invariant observables are also experimentally accessible. An important example of such non-gauge invariant observable is the chirality used in the experiment of references [9, 10] to detect the presence of chiral currents induced by the

Figure 1. (a) Schematic picture of the system considered in this work; \( t \) and \( \Omega \) parametrize the intra- and inter-leg hopping, respectively; \( \phi \) is the applied (synthetic) magnetic flux per plaquette; \( U > 0 \) parametrizes the strength of the repulsive inter-leg interaction. The leg labels are \( \sigma = \uparrow \) (upper leg) or \( \sigma = \downarrow \) (lower leg). (b) The four possible types of band structure depending on the flux and the ratio \( \Omega/t \) for non-interacting particles (see appendix B). The horizontal (vertical) lines in subfigures A–D correspond to zero energy (momentum). The band structures are centered at wave number \( q = -\phi / \pi \). For the different types of band structure, we used the notations introduced in reference [23]. In the phase diagram, \( \phi_\uparrow (\phi_\downarrow) \) denotes the flux for which a double-well (band gap) appear in the band structure. Note that the D phase has only two Fermi points independently of the lattice filling. However, the C phase can have more than two, and, in particular, for \( \phi = \pi \) it always has four Fermi points for any lattice filling \( n < 1 \). The red line corresponds to the value of \( \Omega/t \) realized in the experiment of reference [9].
synthetic gauge field. In the setup of references [9, 10] a particular gauge choice where \( \phi_1 = \phi \) and \( \phi_\uparrow = 0 \) is realized. The chirality is mathematically defined as:

\[
C = \int_{-\pi}^{+\pi} \frac{dq}{2\pi} n_\uparrow(q) \text{sign}(q),
\]

where \( n_\uparrow(q) = \langle c_\uparrow^\dagger c_\uparrow \rangle \) (with \( c_{\sigma,\uparrow} = L^{-1/2} \sum_m e^{imq} c_m \)) is the momentum distribution of the \( \uparrow \) fermions. Note that the momentum distribution \( n_\uparrow(q) \) and therefore the chirality \( C \) in equation (8) are not invariant under gauge transformations such like equation (5). This means that they have no counter-part in condensed matter systems which can be emulated using this atomic system.

However, a gauge invariant quantity can be defined and measured if we replace the \( \text{sign}(q) \) function in equation (8) by a (shifted) \( \sin \) function:

\[
\tilde{C}(\phi) = \int_{-\pi}^{+\pi} \frac{dq}{2\pi} n_\uparrow(q) \sin(q + \phi).
\]

In the gauge choice used by the experiment this quantity is related to the derivative of the energy with respect to the flux \( \phi_1 = \phi \) (cf equation (19))

\[
2t\tilde{C}(\phi) = \frac{1}{L} \left\langle \frac{\partial H}{\partial \phi_1} \right\rangle = \frac{1}{L} \left\langle \frac{\partial H}{\partial \phi} \right\rangle.
\]

The latter derivative is gauge invariant and therefore does not depend on \( \phi_1 \) and \( \phi_\uparrow \) separately but only on their difference \( \phi = \phi_1 - \phi_\uparrow \). Indeed, for a general gauge choice, it is proportional to the orbital current per unit length:

\[
\frac{J(\phi)}{L} = - \frac{1}{L} \left\langle \frac{\partial H}{\partial \phi} \right\rangle = -2t\tilde{C}(\phi),
\]

which is the observable on which we shall focus our attention below. Thus, we emphasize that, since the chirality is can be accessed in the experiments of references [9, 10], the orbital current is also measurable. Indeed, both quantities are related to the momentum distribution of the atoms in the \( \sigma = \uparrow \) internal state in the particular gauge choice implemented in references [9, 10].

### 3. Orbital currents

In ultracold atom systems, unlike many condensed matter systems, as the flux per plaquette \( \phi \) is varied, the particle number (and not the chemical potential) remains constant. Thus, in this section, we describe the calculation of the orbital current and the orbital susceptibility at fixed particle number. Although in our numerical and analytical calculations we have restricted ourselves to zero temperature, it is useful to discuss the finite temperature case. In what follows, we set Boltzmann’s constant \( k_B = 1 \) and denote the inverse absolute temperature by \( \beta (= T^{-1}) \).

Let us first consider the partition function in the grand canonical ensemble:

\[
Z(\beta, \mu, \phi) = \text{Tr} \left[ e^{-\beta \left( H(\phi) - \mu N \right)} \right],
\]

where \( \mu \) is the chemical potential. In condensed matter systems at fixed \( \mu \), the orbital current is defined as a derivative of the grand canonical potential, i.e.

\[
\Omega(\beta, \mu, \phi) = - \frac{1}{\beta} \log Z(\beta, \mu, \phi),
\]

\[
J(\mu, \phi) = \left\langle \frac{\partial \Omega(\beta, \mu, \phi)}{\partial \phi} \right\rangle_{\beta, \mu}
\]

\[
= \frac{\text{Tr} \left[ e^{-\beta \left( H(\phi) - \mu N \right)} \hat{J}(\phi) \right]}{Z(\beta, \mu, \phi)}
\]

\[
= \langle \hat{J}(\phi) \rangle_{\beta, \mu},
\]

where

\[
\hat{J}(\phi) = \frac{\partial \hat{H}(\phi)}{\partial \phi}
\]
Hence, the orbital current for a fixed particle number can be obtained from the free energy,

\[ J = \frac{1}{\beta} \sum_{m, \sigma} \frac{d \phi_m}{d \phi} \left[ e^{\phi_m} c^\dagger_{m, \sigma} c_{m+1, \sigma} - \text{h.c.} \right] \tag{18} \]

\[ = -2t \sum_{q \in 1BZ, \sigma} \left( \frac{d \phi_q}{d \phi} \right) \sin \left( q + \phi_\sigma \right) c^\dagger_q c_\sigma \tag{19} \]

is the orbital current operator and 1BZ stands for the 1st Brillouin zone, which corresponds to the segment \((-\pi, \pi]\).

However, we are interested in the current \( J(N, \phi) \) at fixed particle number \( N \). In order to obtain the latter, we can start from the constraint equation for the particle number \( N \):

\[ N = \langle \hat{N} \rangle = -\frac{\partial \Omega(\beta, \mu, \phi)}{\partial \mu} \beta, \phi = N(\beta, \mu, \phi). \tag{20} \]

By solving this equation for \( \mu = \mu(\beta, N, \phi) \) and introducing the solution into \( \tilde{J}(\beta, \mu, \phi) \) we obtain the orbital current \( J(\beta, N, \phi) \) as a function of \( N \).

Alternatively, we can work with the thermodynamic potential that is the Legendre transform of the Grand canonical potential \( \Omega(\beta, \mu, \phi) \), i.e.,

\[ G(\beta, N, \phi) = \Omega(\beta, \mu(\beta, N, \phi), \phi) + \mu(\beta, N, \phi)N. \tag{21} \]

Hence, the orbital current for a fixed particle number can be obtained from the free energy,

\[ G(N, \phi) = -\frac{1}{\beta} \log Z(\phi) + \mu(\phi)N \tag{22} \]

as a derivative:

\[ J(N, \phi) = -\left[ \frac{\partial}{\partial \phi} G(\beta, N, \phi) \right]_{\beta, N} \tag{23} \]

\[ = \frac{\text{Tr} \left[ e^{-\beta(\hat{H}(\phi) - \mu(\beta, N, \phi))} \right] (\phi)}{Z(\beta, \mu(\beta, N, \phi), \phi)} \tag{24} \]

\[ = \langle J(\phi) \rangle_N. \tag{25} \]

Another quantity of interest is the orbital susceptibility, which is defined from the derivative of the orbital current density with respect to \( \phi \):

\[ \chi(\beta, N, \phi) = \left[ \frac{\partial}{\partial \phi} \frac{J(\beta, N, \phi)}{L} \right]_{\beta, N} \tag{26} \]

\[ = -\frac{1}{L} \left[ \frac{\partial^2}{\partial \phi^2} G(\beta, N, \phi) \right]_{\beta, N}. \tag{27} \]

Note that, at the zero temperature \( (T = 0) \), the thermodynamic potential \( G(\beta, N, \phi) \) becomes the ground state energy calculated at fixed particle number \( N \). Likewise, at \( T = 0 \) the expectation of equation (17) is taken over the ground state of the system containing \( N \) particles. In the DMRG calculations of \( J(N, \phi) \) that are described in the following section, the constant particle number constraint is imposed by projecting the ground state on the subspace of the Hilbert space with total particle number equal to \( N \) (the latter is determined by the system length \( L \) and the lattice filling \( n = N/L \)).

To illustrate the differences between the orbital current and susceptibility computed at fixed particle number and chemical potential, we have plotted them in figure 2. The chemical potential at \( \phi = 0 \) has been chosen to yield a lattice filling of \( n = 0.75 \), which is the same value used for the calculations at fixed particle number. Thus, although the curves for the orbital current and the susceptibility are very close at small \( \phi \), they show large deviations for \( \phi \approx \frac{\pi}{2} \). The difference can be understood from the changes in the band occupation in the cases of fixed \( n \) and fixed \( \mu \); whereas at fixed \( n = 0.75 \) the system transitions from a metal with two Fermi points to a metal with four Fermi points, for constant \( \mu \) the system transitions from a metal to a band insulator as the chemical potential moves into the band gap with \( \phi \) increasing from 0 to \( \pi \). At the transition points, the orbital current shows a cusp and the susceptibility becomes singular. However, beyond the cusp, the curves at fixed \( \mu \) for both the orbital current and the susceptibility fall on top of the curves with constant lattice filling \( n = 1 \) (dashed curves). For the latter filling the system is a band insulator at any \( \phi \) for large \( \Omega \). Thus, to sum up, whilst the system at fixed lattice filling exhibits a transition between two
different metallic phases, for fixed chemical potential it undergoes a transition from a metal with two Fermi points to a band insulator. The singular behavior of the susceptibility is different for the two kinds of constraints. The different types of singularities are analytically calculated in appendix C. We find that, for a non-interacting system with fixed particle number, the orbital susceptibility has a step-like discontinuity. On the other hand, $(\phi - \phi_c)^{-1/2}$ singularities are found for fixed chemical potential.

To further explore the dependence on the lattice filling in the non-interacting case, in figure 3 we have plotted the current at different values of $n$. Note that the orbital current vanishes both at $\phi = 0$ and $\phi = \pi$. In the latter case, the hopping amplitudes are all real but the unit cell size doubles (to see this, notice that, e.g. in the gauge choice of equation (1), the phase of the inter-leg hopping in $H_1$, equation (3) becomes $(-1)^j$ for $\phi = \pi$). In addition, in all cases shown in figure 3, the orbital current reaches a maximum and exhibits a cusp as $\phi$ changes from 0 to $\pi$. As for the case where $n = 0.75$ studied above, this happens when the system undergoes a topological Lifshitz transition where the number of Fermi points changes. The transition is also reflected in the orbital susceptibility as a divergence (see appendix C). Below, we shall see that the cusp in the orbital current persists in the presence of interactions. This observation strongly suggest that at least some of the interaction effects can be captured by a properly renormalized (mean-field) band structure as we show in section 4.3.

4. Interaction effects

4.1. Limit of large inter-leg hopping

The two-leg ladder model introduced in section 2 contains three different energy scales $t$, $\Omega$ and $U$. In order to appreciate the importance of the interaction in the limit where $\Omega$ is the largest of the three energy scales, let us fix first the Gauge to the symmetric gauge where $\phi_1 = -\phi_\perp = \phi/2$. For large $\Omega > 0$, it is convenient to diagonalize the inter-leg hopping term by means of a unitary spin rotation:

\[
\begin{pmatrix}
\epsilon_{m\uparrow} \\
\epsilon_{m\downarrow}
\end{pmatrix}
= \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix}
\begin{pmatrix}
\epsilon_{m\uparrow} \\
\epsilon_{m\downarrow}
\end{pmatrix},
\]

(28)
Thus, \[
H_\perp = -\frac{\Omega}{2} \sum_m \left(c_{m,\downarrow}c_{m+\downarrow} - c_{m,\uparrow}c_{m+\uparrow}\right)
\] (29)
and the lowest energy state at a given site \(m\) is \(|\rightarrow\rangle_m = c_{m,\uparrow}^\dagger |0\rangle\), which is separated by gap equal to \(\Omega\) from the \(|\leftarrow\rangle_m = c_{m,\downarrow}^\dagger |0\rangle\) state.

Let us next consider the interaction term, \(H_U\). When performing the above spin rotation, it is useful to write it in a rotational invariant fashion, in terms of the total site occupation \(n_m = n_m^\uparrow + n_m^\downarrow = n_m,\uparrow + n_m,\downarrow\). Hence, it follows that \(H_U\) remains unchanged:

\[
H_U = U \sum_m n_m^\uparrow n_m^\downarrow
\]
(30)
\[
= \frac{U}{2} \sum_m (n_m - 1)^2 + \frac{U}{2} N - \frac{UL}{2}
\]
(31)
\[
= \frac{U}{2} \sum_m n_m - n_{m,\uparrow} n_{m,\downarrow}.
\]
(32)

For \(t = 0\) and lattice filling \(n \leq 1\), the above expressions imply that repulsive interactions play no role in the ground state as all sites can be either occupied with a single fermion in the \(|\rightarrow\rangle_m\) level or be empty (i.e. \(|0\rangle_m\)). Thus, as long as \(n \leq 1\) and \(t = 0\), the many-particle states in this subspace are all degenerate in energy. This large degeneracy is lifted by the hopping term, \(H_t\), which, in the new basis, takes the form:

\[
H_t = -\sum_m \left(c_{m+1,\uparrow}^\dagger c_{m,\uparrow} + c_{m,\downarrow}^\dagger c_{m+1,\downarrow}\right) \mathcal{T}(\phi) \left(c_{m,\uparrow} c_{m,\downarrow}^\dagger\right) + \text{h.c.}
\]
(33)
\[
\mathcal{T}(\phi) = \begin{pmatrix} \cos \phi/2 & i \sin \phi/2 \\ i \sin \phi/2 & \cos \phi/2 \end{pmatrix}.
\]
(34)

Note that the price to pay for working with \(\{c_{m,\uparrow}, c_{m,\downarrow}\}\) is a non-diagonal \(H_t\). For fermions in the low-lying \(\rightarrow\) level and as long as \(t \ll \Omega\), the hopping amplitude becomes \(t \cos \phi/2\) and we are left with a band with a modified dispersion:

\[
\tilde{\epsilon}_q = -2t \cos(\phi/2) \cos q.
\]
(35)

Thus, we can regard the system at filling \(n < 1\) as a ferromagnetic (or spin-polarized) metal with weak interactions as long as \(|U| \ll \Omega\). Weak effective interactions are introduced by virtual hopping processes mediated by the off-diagonal terms of \(H_t\), which admix the \(\rightarrow\) and \(\leftarrow\) levels thus allowing the fermions to interact. Note that this weakly interacting metal does not have a charge gap but it still has a spin gap \(\tilde{\epsilon}_q \approx \Omega > U\), which is the energy cost to flip one spin from \(\rightarrow\) to \(\leftarrow\). Thus, with the possible exception of half-filling, we can regard the system as a spin-polarized weakly correlated Tomonaga–Luttinger liquid [20] (see also discussion in section 4.4 below).

Nevertheless, the simple picture provided above runs into trouble because the (lowest) band flattens for \(\phi \rightarrow \pi\) since its width decreases as \(w = 4t \cos \phi/2\). At the same time, the magnitude of the off-diagonal spin-flip hopping terms in \(H_t\) grows. This results in an increase of the admixture between the \(\rightarrow\) and \(\leftarrow\) levels. Thus, for \(\phi \gtrsim \pi/2\), interaction effects are expected to become more important. This expectation is confirmed by the DMRG results for the orbital current discussed below (see e.g. figure 5 and the discussion in the next subsection).

Nevertheless, we also find instances at small \(\phi\) for which the behavior of the orbital current can be substantially altered by interactions (cf figure 4). This can be understood as follows: even in the absence of interactions, the orbital susceptibility at \(\phi \rightarrow 0\) is not entirely determined by the dispersion in (35) but also depends on the admixture of the \(\rightarrow\) and \(\leftarrow\) levels. This admixture is responsible for the sign of the orbital susceptibility \(\phi = 0\) (see figure 3 as well as equation (B4) in appendix B2). As noted above, the admixture also allows fermions to interact. Therefore, as \(U\) increases, the orbital susceptibility at small \(\phi\) gets renormalized in a rather dramatic way by changing sign: the system undergoes a transition from diamagnetic to paramagnetic behavior (cf figure 4). Note that such a change of behavior is suppressed by a sufficiently large \(\Omega\) as also shown on the right panel of figure 4.

4.2. DMRG results
We have carried out DMRG calculations using the ALPS Library [33, 34] for systems up to \(L = 128\) sites, using up to 128 block states. We have checked the convergence with both system size \(L\) and number of DMRG block states. In addition, for the non-interacting case, we have found that the results for the orbital current for \(L = 128\) and \(m = 128\) are, for most points, within less than 1% of the exact results in the...
Figure 4. Effect of inter-chain (i.e. inter-species) interaction on the orbital current obtained from DMRG. The lattice filling is $n = 0.75$ and two values of the inter-chain hopping are shown: $\Omega = 4.28t$, which is the value in the experiment of reference [9] and $\Omega = 10t$. DMRG results are shown as dots. The dashed lines are a guide to the eye. Panel (a) shows that interactions can drive a transition from diamagnetic to paramagnetic behavior. We define diamagnetic (paramagnetic) behavior by the negative (positive) orbital susceptibility at $\phi = 0$, i.e. the slope of the orbital current at small $\phi$. Note that, as shown on panel (b), no paramagnetic-diamagnetic transition occurs for the larger value of $\Omega = 10t$. As explained in the main text, the overall effect of interaction becomes weaker for larger $\Omega$.

Figure 5. DMRG results for the orbital current (upper panels, (a)) and the deviation from the non-interacting orbital current (lower panels, (b)) for several values of the inter-leg interaction $U$ and the inter-leg hopping $\Omega$ with lattice filling $n = 0.25$. (a) At this lower lattice filling, the overall effect of inter-leg interaction on the orbital current is weaker and, in agreement with the results shown figure 4, it is further suppressed at larger $\Omega/t$. To show the effects of the interaction more clearly, we have also plotted the deviation of the orbital current from the non-interacting limit. Note the interaction effects are more important for $\phi$ larger than the flux value for which the orbital current exhibits a cusp.

This provides an estimate of the finite-size error. Full details about the numerical convergence of the results are provided in appendix E (cf especially figure 16).

Figures 4 and 5 show our DMRG results for the orbital current for two values of the inter-leg hopping $\Omega/t = 4.28$ and $\Omega/t = 10$ ($\Omega/t = 4.28$ corresponds to the experimental value [9]), two values of the lattice filling, $n = 0.75$ and $n = 0.25$, and for $U$ ranging from zero to $10t$. Note the presence of a cusp in all curves of the orbital current as $\phi$ approaches $\pi$. The latter is already present in the non-interacting case (i.e. $U = 0$) and corresponds, as explained above, to a topological quantum phase transition where the number of Fermi points in the lower band changes from two to four Fermi points. Generally speaking, the position of the cusp is pushed towards slightly larger values of $\phi$ as the strength of $U$ increases. This effect is more noticeable for the smaller $\Omega$ and the larger lattice filling $n$ (cf figure 4, panel (a)), for which interactions have a more pronounced effect (see below).

Another noticeable effect is that repulsive interactions tend to enhance the orbital current (see lower panels of figure 5). This is precisely the opposite of what is expected for attractive interactions, for which fermions on different legs (i.e. different pseudo-spins) tend to form pairs for sufficiently large negative $U$, which would suppress the orbital (or pseudo-spin) current. Furthermore, as mentioned above, for the smaller value of $\Omega/t$ and for small values of $\phi$, this enhancement can actually reverse the slope of the orbital current at $\phi = 0$, thus inducing a transition from ‘paramagnetic’ behavior (characterized by an orbital susceptibility $\chi < 0$ at zero field) to ‘diamagnetic’ behavior (for which $\chi > 0$ at $\phi = 0$), see figures 3 and 4 and appendix B2. Figure 5 shows the orbital current and its deviation from the non-interacting case using DMRG computations at low filling $n = 0.25$. In the limit of low density and large $\Omega$, the effect of interaction is weak (<10% for $U$ up to $10t$). Note as well that the orbital current appears to be more sensitive to interaction effects beyond the cusp. Some of the observed trends in the DMRG results can be qualitatively understood from the following reasoning: since the interaction energy per unit length is of order $\sim Un^2/4$ whereas in the large $\Omega$ limit the kinetic term is $\sim \Omega n + O(t)$, the importance of the interaction effects can be estimated from the ratio $\sim Un/\Omega$, which decreases with lattice filling and larger $\Omega$. 

thermodynamic limit. This provides an estimate of the finite-size error. Full details about the numerical convergence of the results are provided in appendix E (cf especially figure 16).
4.3. Mean-field theory

In the previous section, using essentially numerically exact DMRG calculations, we have shown that the orbital current of the interacting system retains many features of the non-interacting orbital current, in particular it exhibits a cusp as $\phi$ approaches $\pi$. This result strongly suggests that a conveniently renormalized mean-field band structure will describe this behavior. In this section, such mean-field theory is developed for $U > 0$.

In order to apply mean-field theory to the model Hamiltonian introduced in section 2, we define the following fluctuation operators:

$$\delta \hat{\alpha}_m = \hat{\alpha}_m - \alpha_m(\phi),$$

$$\delta \hat{n}_{m,\sigma} = \hat{n}_{m,\sigma} - n_{m,\sigma}(\phi),$$

where $\delta \hat{\alpha}_m = c_{m,\uparrow}^\dagger c_{m,\downarrow}$. The order parameters (see appendix D for details of their numerical evaluation in finite systems) are:

$$\alpha_m(\phi) = \langle \delta \hat{\alpha}_m \rangle = \langle c_{m,\uparrow}^\dagger c_{m,\downarrow} \rangle,$$

$$\langle \delta \hat{n}_{m,\sigma} \rangle = n_{m,\sigma}(\phi).$$

Note that the constraint of constant particle number requires that

$$\sum_m [n_{m,\uparrow}(\phi) + n_{m,\downarrow}(\phi)] = N. \tag{39}$$

In the mean-field approximation where the fluctuation energy is neglected (i.e. terms that are quadratic in the operators $\delta \hat{\alpha}(j)$ and $\delta \hat{n}_{m,\sigma}$ are thrown away), the interaction term becomes

$$U^{MF} = \sum_{m} \left[ -n_{m,\uparrow}n_{m,\downarrow} + n_{m,\uparrow}c_{m,\uparrow}^\dagger c_{m,\downarrow} + n_{m,\downarrow}c_{m,\downarrow}^\dagger c_{m,\uparrow} + U \sum_m \left[ (\alpha_m(\phi))^2 - \alpha_m(\phi)c_{m,\uparrow}^\dagger c_{m,\uparrow} + \alpha_m(\phi)c_{m,\downarrow}^\dagger c_{m,\downarrow} \right] \right]. \tag{40}$$

This expression allows us to write the mean-field Hamiltonian as follows:

$$H^{MF} = H_0 + U^{MF}. \tag{41}$$

In order to be able to compare to the DMRG data, we have diagonalized the mean-field Hamiltonian (41) numerically in chains of length up to 128 sites with open boundary conditions. The order parameters are obtained self-consistently by solving the mean-field equation (38) (see appendix D for details). Using the self-consistent solution, we have obtained the orbital current that is shown in figure 8. Numerically, we find that $n_{m,\uparrow} \approx n_{m,\downarrow}$ and therefore the only effect of the inter-leg interaction is to enhance the inter-leg hopping by renormalizing it to larger (average) value: $\Omega(\phi) = 2U\alpha(\phi) + \Omega$. The mean-field enhancement of the inter-leg hopping (cf figure 6) can be qualitatively understood by realizing that, for repulsive interactions, configurations such as the one shown in figure 7 are favored by both the inter-leg hopping ($\propto U$ in equation (1)) and the interactions ($\propto U$ in equation (1)). The renormalization of the inter-leg hopping also qualitatively explains the enhancement of the orbital current, as a larger effective $\Omega$ makes it easier for the fermions to circulate around the plaquettes.

Figure 8 shows the comparison between the mean-field theory, perturbation theory (see appendix A1), and the DMRG results for $n = 0.75$, $\Omega = 4.28t$ as a function of $\phi/\pi$ (figure 8). Note that the leading order perturbation theory is accurate as long as $4Ut^2 \sin^2(\phi/2)/\Omega^3 \ll 1$ and over the considered parameter range is the less accurate of the three approaches compared in figure 8. Mean-field theory is most accurate for $U/\Omega \lesssim 1$. Figure 9 shows the comparison of the energy and current obtained within the mean-field theory and DMRG for $n = 0.75$, $\Omega = 4.28$, $\phi = \pi/2$ as a function of $U/t$. In the large $U$ limit, the energy density and orbital current appear to saturate with increasing $U/t$. The limiting values at large $U$ are not fully captured by the mean-field theory, which is due to correlation effects that are neglected within the approach (see also section 4.5 below). Thus, for a completely accurate calculation of the orbital current in the regime $U \gg \Omega = 4.28t$, we must entirely rely on DMRG.

Based on the numerical observation that mean-field theory accurately reproduces both the energy and the orbital current for $U \lesssim \Omega$, we have obtained the mean-field phase diagram shown in figure 10. The boundaries of the phase diagram are calculated by locating the changes of sign and singularities of the orbital susceptibility $\chi(\phi, n)$, which can be also obtained from the mean-field theory. Thus, we find a decrease in size of the diamagnetic region as the strength of $U$ is increased (cf figure 10).
Figure 6. (Average) mean-field renormalized inter-leg hopping $\Omega$ as a function of the inter-leg strength $U/t$. In a system with open boundary conditions, the order parameter $\alpha_m(\phi) = \langle c_m^\dagger, c_m \rangle$ is not uniform. Here we have plotted the average $\alpha = \sum_m \alpha_m(\phi)/L$.

Figure 7. One of the possible ground-state configurations in the large $U > 0$ and large inter-leg hopping, where all the occupied sites have no neighboring sites in the other chain occupied.

Figure 8. Comparison of different theoretical approaches to compute the current for different interaction strengths. The inter-leg hopping is $\Omega = 4.28t$, and filling $n = 0.75$. The DMRG results is derived using system size $L = 128$ and states $m = 128$, which is well-converged. The DMRG results match the mean-field result for interaction strength $U$ up to $\sim \Omega$.

zero field can be also understood by using the mean-field renormalized inter-leg hopping $\Omega(\phi)$ in equation (B4) from the appendix.

In addition, in figure 10, we have used a dashed line to indicate the phases available for $n = 0.75$ and $\phi = 0.95\pi$ for different values of $U$, so that comparison with the upper-left panel of figures 11 and 12 is possible. Notice that, for this lattice filling and flux, mean-field theory predicts an interaction-driven Lifshitz transition between four and two Fermi points phases. This result is consistent with the cusps in the orbital current observed in the DMRG results on figure 11 (panel (a)), which shows a cusp in the orbital current for $U/t \simeq 4$ (see also following section). On figure 11 we also show the behavior of the orbital current for $n = 1$, for which the system is a fully gapped ferromagnetic insulator. In this phase, the orbital current changes smoothly with increasing $U/t$ and $\phi$ and no cusps in the current are observed as no Lifshitz transitions can occur.

4.4. Interaction-induced Lifshitz transition

Finally, let us briefly discuss the limit of $U \gg t, \Omega$ close to unit lattice filling. In this parameter regime, the intra-chain hopping $H_I$ is the smallest term in the Hamiltonian. Second order perturbation theory at unit filling allows to map the Hamiltonian onto a spin-chain model with Dzyaloshinskii–Moriya interactions in a transverse magnetic field $\propto \Omega$ [22]. Let us recall that for $\Omega = 0, \phi = 0$, the system is a
Figure 9. Comparison of mean-field theory and DMRG: (a) energy density as a function of the inter-leg interaction strength $U/t$ for $\Omega/t = 4.28$ ($t$ is the intra-leg hopping), $\phi = \pi/2$, and $n = 0.75$. Mean-field theory is accurate up to $U \sim \Omega$. At saturation of the orbital current is observed at large $U$, which is not well captured by the present mean-field theory.

Figure 10. Mean-field phase diagram for $\Omega = 4.28t$ and different values of the interaction strength $U$. The mean-field theory described in section 4.3 is accurate for $U \lesssim \Omega$. The dashed line indicates the lattice filling $n = 0.75$ used in the upper panel in figure 8. The interaction $U$ enhances the paramagnetic behavior in the two Fermi-point metallic phase, which is overall rendered more stable by interactions. In this regard, note the mean-field theory predicts that for $n = 0.75$ and $\phi = 0.95\pi$ the system undergoes a Lifshitz phase transition driven by the interaction at $U \simeq 4t$, which is confirmed by our numerically exact DMRG calculations (see figure 11 and also figure 12). The value $\phi$ at which ‘double well’ bands appear, $\phi_0$, is also indicated, see also figure 1.

Figure 11. Interaction-induced topological Lifshitz transition from DMRG. (a) Dependence of the current density on the interaction strength $U$ for a metallic lattice filling of $n = 0.75$. Note there is a cusp in orbital current for $\phi = 0.95\pi$, which can be understood as an interaction-induced topological Lifshitz transition from a four Fermi-point to two Fermi-point metal with increasing $U/t$ (see section 4.4 and figure 12). (b) Dependence of the energy density on $U$ for $n = 0.75$. Note that both the energy and its derivative, i.e. the orbital current, appear to saturate at large $U$. (c) Dependence of the current density on $U$ for the insulating filling $n = 1$. (d) Dependence of the energy density on $U$ for $n = 1$ filling. At this filling, the system is a band insulator. Note the absence of a cusp for any value of $\phi$, and the difference with the metallic case at $n = 0.75$. There are no Lifshitz transitions for this insulating filling.

Tomonaga–Luttinger liquid with charge gap but no spin gap [20]. For $\phi, \Omega \neq 0$, as obtained in reference [35] (in the uncoupled chain limit corresponding to $J_\perp = 0$ in the notation of that article), the spin chain undergoes a commensurate–incommensurate phase transition from the spin-gapless Tomonaga–Luttinger to a fully gapped ferromagnetic insulator [22]. Although to the best of our knowledge, there is no analytical expression for the critical curve $\Omega_c(\phi)$, $\Omega_c \lesssim 4t^2/U$ for all $\phi$ being $\Omega_c = 0$ for $\phi = \pi/2$ [35]. Furthermore,
since the mapping to a spin chain requires that $U \gg t$, $\Omega_\epsilon$ is therefore small and lies outside the large $\Omega$ regime studied in this article.

Nevertheless, in the large $U$ and $\Omega$ limit, it is tempting to regard the system at $n \lesssim 1$ as a ferromagnetic metal resulting from doping a ferromagnetic insulator that is adiabatically connected to the one described in reference [35]. In mean-field theory, this ferromagnetic metal has the band structure described in section 4.3, and thus exhibits a large spin gap of the order of the renormalized inter-leg hopping $U/t = 3, 5$. Unlike the non-interacting case, the intensity of the spectrum obtained from mean-field theory differs from the DMRG result, which is due to correlation effects. However, notice that the position of the peaks is the same for mean-field theory and DMRG. Panel (c) shows the system is in a metallic phase with only two Fermi points for $U/t = 3$ and therefore the spectrum shows a single peak at $q = (2\pi - 2k)$. The Fourier spectrum in all panels is $2\pi$ periodic and symmetric with respect to $q = 0$ with the Fourier components at $q = 0$ vanishing by Kirchhoff's law. The peaks at wave numbers $q_1, q_2, q_3, q_4$ must be folded within the first Brillouin zone, which is chosen to be $(-\pi, +\pi]$.

![Figure 12](image.png)

Figure 12. (a) Absolute value of the Fourier components of the inter-leg current $j_{\parallel}^{m}(\phi)$ for particle filling $n = 0.75$ and $\phi = 0.85\pi$ computed using DMRG (dashed line) and exact diagonalization at $U/t = 0$ (continuous line). The curves exhibit peaks located at wave numbers $q_1 = k_{22} - k_{11}, q_2 = k_{12} + k_{12}, q_3 = 2k_{22}$, and $q_4 = 2k_{11}$, where $\pm k_{11}$ and $\pm k_{22}$ are the Fermi momenta in the four Fermi-point phase. (b) and (c) Same quantity for inter-leg interaction strength $U/t = 3, 5$. Unlike the non-interacting case, the intensity of the spectrum obtained from mean-field theory differs from the DMRG result, which is due to correlation effects. However, notice that the position of the peaks is the same for mean-field theory and DMRG. Panel (c) shows the system is in a metallic phase with only two Fermi points for $U/t = 3$ and therefore the spectrum shows a single peak at $q = (2\pi - 2k)$. The Fourier spectrum in all panels is $2\pi$ periodic and symmetric with respect to $q = 0$ with the Fourier components at $q = 0$ vanishing by Kirchhoff's law. The peaks at wave numbers $q_1, q_2, q_3, q_4$ must be folded within the first Brillouin zone, which is chosen to be $(-\pi, +\pi]$.

The continuum-limit representation of the fermion operator for the lower (partially-filled) band with four Fermi points:

$$c_{m,\sigma} \sim A_{RL,\sigma} \psi_{R_{L},\sigma}^{\dagger}(x_m) e^{-i k_{L} x_m} + A_{R2,\sigma} \psi_{R_{2},\sigma}^{\dagger}(x_m) e^{i k_{2} x_m} + A_{L1,\sigma} \psi_{L_{1},\sigma}^{\dagger}(x_m) e^{i k_{1} x_m} + A_{L2,\sigma} \psi_{L_{2},\sigma}^{\dagger}(x_m) e^{-i k_{2} x_m},$$

(42)

where $x_m = m$ and $\psi_{RL,1/2}(x)$ are Fermi fields that vary slowly on the scale of the lattice and describe the low-energy degrees of freedom of the system [20]. The coefficients $A_{RL,\sigma}, A_{L1,\sigma}$ are related to the angle $\theta(q, \phi)$ introduced when diagonalizing the kinetic energy (see equation (A6) in appendix A). Thus, the
continuum limit of the intra-leg interaction, equation (4) contains the following two types of scattering processes between the two sets of Fermi points in the lower band:

\[ H_U = H_+ + H_- + \cdots \]  

(43)

\[ H_+ = g_+ \int dx \psi_{R1}^\dagger(x) \psi_{L2}^\dagger(x) \psi_{L2}(x) \psi_{R1}(x) + \text{h.c.} \]  

(44)

\[ H_- = g_- \int dx \psi_{L1}^\dagger(x) \psi_{R1}^\dagger(x) \psi_{L2}(x) \psi_{R2}(x) + \text{h.c.} \]  

(45)

The ellipsis in equation (43) stands for forward scattering and other terms that (for arbitrary fillings) oscillate rapidly on the lattice scale. The interactions described by \( H_+ \) correspond to processes for which a fermion is scattered by another fermion from one Fermi point to another by exchanging a momentum \( k_{f2} \pm k_{f1} \) (recall that \( k_{f2} - k_{f1} = \pi n \) but the individual values of \( k_{f1,2} \) depend on the band dispersion). These scattering processes can potentially become relevant perturbations in the renormalization-group (RG) sense, which would result in the gapping some of the low-energy degrees of freedom of the four Fermi-point metal. However, note that \( H_- \) is obtained by exchanging the final states in \( H_+ \). Hence, the relation \( H_- = -g_- H_+/g_+ \) follows. In addition, the coupling constants \( g_{\pm} = A_{R1} A_{R2} A_{L1} A_{L2} U \) in the small \( U \) limit and therefore, for the type of interactions considered here, \( H_- \) appears to cancel \( H_+ \) in the weak coupling limit. A more detailed perturbative analysis for general interactions of the flow of the \( g_{\pm} \) couplings under RG scaling is beyond the scope of this work and will be presented elsewhere [36].

We have also attempted to numerically address the issue of the existence of a correlation gap in the four Fermi-point phase at finite \( U \) by computing the central charge of the system from the scaling of the subsystem entanglement entropy, which is one of the outputs of the DMRG code. We have found strong evidence that the central charge of the metallic phase across the Lifshitz transition shown in figure 11(a) (i.e. for \( U/t = 5, \phi = 0.95\pi, \) and \( n = 0.75 \)) is \( c = 1 \), as corresponds to a two Fermi-point metal. However, the situation is less clear for \( U/t \lesssim 4 \), for which \( c = 2 \) is expected. This is because the entanglement entropy shows rather pronounced oscillations [37] as a function of the subsystem size. Even after extending our calculations up to \( L = 512 \) sites and \( m = 512 \) states, we were unable to reach a definite conclusion on the central charge of the metallic phase on the small \( U/t \) side of the transition for \( \phi = 0.95\pi \) and \( n = 0.75 \).

However, let us point out that the DMRG results discussed in the following section for the Friedel oscillations of the inter-leg current appear to be consistent with the absence of a interaction-induced gap.

### 4.5. Friedel oscillations of the inter-leg current

So far, we have discussed the behavior of the average orbital current density using DMRG, mean-field theory, and perturbation theory. As described in the previous section, mean-field theory deviates from DMRG in the strongly interacting limit (cf figure 8), where it fails to fully capture saturation of both the energy and current densities. Besides this, as we show below, the decay of the oscillations of the inter-leg current also is not correctly reproduced by the mean-field approach for finite \( U \). The inter-leg current is defined by the (ground-state expectation value of the) imaginary part of the inter-leg hopping operator, i.e.

\[ j_\perp(m) = \frac{\Omega}{2} \text{Im} \left[ \langle \hat{c}_{m\uparrow} \right] = -\frac{\Omega}{2} \text{Im} \left[ \langle \gamma_{m\uparrow} \gamma_{m\downarrow} \rangle \right]. \]  

(46)

In lattices with periodic boundary conditions, translational invariance implies that \( j_\perp(m) \) is a constant independent of \( m \), which vanishes by Kirchhoff’s laws. However, because in our mean-field and DMRG calculations are carried out in systems with open boundary conditions, \( j_\perp(m) \) displays (Friedel) oscillations near the boundaries as described below.

In order to characterize the oscillatory behavior of the inter-leg current, we have computed its Fourier transform defined as:

\[ F [j_\perp](q) = \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{iqm} j_\perp(m). \]  

(47)

In figure 12, we have plotted the absolute value of the Fourier components of the inter-leg current obtained from DMRG and mean-field theory for \( n = 0.75 \) and \( \phi = 0.95\pi \). We notice that for \( U/t = 0 \) and \( U/t = 3 \) (left panel), the spectrum displays singularities at a set of wave numbers that correspond to \( q_{1} = k_{f1} + k_{f2}, q_{2} = k_{f2} - k_{f1}, q_{3} = 2k_{f2}, q_{4} = 2k_{f1} \) (or, indeed, at the corresponding values folded into the positive part of the 1BZ, because \( F [j_\perp](q) \) is periodic with periodicity \( 2\pi \)). These singularities are a consequence of the reflection of fermions at the boundaries, which leads to Friedel oscillations in \( j_\perp(m) \). The wave numbers of the oscillations can be obtained by introducing the low-energy expansion of the fermion operator around the four Fermi points given in equation (42) into equation (46). The behavior of
the Fourier components of the inter-leg current close to these set of wave numbers is related to decay away from the boundaries of the different oscillation harmonics of \( j_{\pm}(m) \) \[23, 38\]. On the other hand, the rightmost panel of figure 12 shows the Fourier spectrum of \( j_{\pm}(m) \) computed at \( U/t = 5 \) from DMRG and mean-field theory. In this case, the singularities are located at \( \pm(2\pi - 2k_F) = \pm0.5\pi \) (recall that \( q = 2k_F = 2\pi n = 1.5\pi \)), as expected for a metallic system with two Fermi points at \( \pm k_F \). These results provide numerical evidence that allows to relate the cusp in the orbital current shown in figure 11 for \( \phi/\pi = 0.95, n = 0.75 \) to an interaction-induced Lifshitz transition from the four to the two-Fermi point phase, as predicted by the mean-field theory.

The central and rightmost panels of figure 12 also show that the mean-field theory fails to reproduce the magnitude of Fourier spectrum of the inter-leg current computed using DMRG results. Indeed, the numerically exact DMRG results display stronger singularities than predicted by the mean-field theory. The latter approach treats particles as independent (i.e. uncorrelated) fermions that move in an effective potential, giving rise to the renormalized inter-leg hopping \( \Omega(\phi) \). In this regard, the (boundary) exponents of the power laws that control the decay of the oscillations away from \( m = 0, L \) are the same as for an non-interacting system. However, as we have mentioned above, the system is a spin-polarized Tomonaga–Luttinger liquid and therefore the boundary exponents are interaction dependent and different from the non-interacting exponents \[20, 23, 38\]. The singularities displayed by the Fourier transform of the inter-leg current are affected by finite-size effects, which complicates the extraction of such boundary exponents. However, qualitatively by eye inspection we observe the peaks in \( F[j_{\pm}](q) \) are more singular than their mean-field (i.e. non-interacting) counterparts.

The presence of these stronger singularities is consistent with the system being gapless on both sides of the interaction-induced Lifshitz transition. Or, if a interaction-induced gap exists in the four Fermi-point phase for \( U/t \lesssim 4 \), the latter remains small for the system sizes of \( L = 128 \) studied here. As mentioned above, additional studies of this issue are necessary and will be reported elsewhere \[36\].

5. Summary, discussion, and outlook

In this work, we have investigated the behavior of the orbital current in a model of a two-leg ladder relevant to ultra-cold gases subject to synthetic gauge fields. We have discussed how the orbital current, which is a gauge invariant observable that can be measured in electronic systems, can be also measured in these atomic setups. In addition, we have seen that, at zero temperature, the orbital current exhibits cusps either as a function of the (pseudo-) gauge flux or the interaction strength. In the non-interacting limit, the cusps can be related to topological Lifshitz transitions, where the number of Fermi points changes. Furthermore, in the non-interacting limit, we have also investigated the analytical form of the singularities in the orbital current and the orbital susceptibility, the latter being the derivative of the orbital current with respect to the flux. Thus, we have found different types of singular behavior depending on whether the particle number or the chemical potential are fixed.

Interestingly, in the presence of repulsive interactions, we have also observed cusps in the orbital current up to values of the interaction strength \( U \) much larger than the inter-leg hopping \( \Omega \), which, as in the experiments \[9, 10\], we have taken to be larger than the intra-leg hopping. For intermediate interactions, i.e. for \( U \lesssim \Omega \), we have shown that mean-field theory is capable of accounting for the cusps in the orbital current. This has allowed us to obtain a mean-field phase diagram by monitoring the changes of sign and singularities of the orbital susceptibility. At small flux per plaquette, we have found that interactions can change the sign of the susceptibility and thus change the behavior of the system from diamagnetic to paramagnetic. At large flux per plaquette, the mean-field theory predicts an interaction induced Lifshitz transition at which the number of Fermi points of the renormalized (mean-field) band structure changes from four to two at fixed particle number. The results obtained from DMRG calculations of the Friedel oscillations of the inter-leg current further support this prediction of mean-field theory.

It is interesting to note that, despite the orbital current being a non-universal quantity that is contributed by all fermions \[22, 23\] (and not only those in the vicinity of the Fermi points), its behavior is very sensitive to the topological properties of the Fermi surface (in the 1D case, the number of Fermi points). Most strikingly, the signatures of Lifshitz transitions discussed above are very robust to the presence of strong interactions. This is perhaps most surprising in the case of the one dimensional systems studied here, for which the concept of ‘band structure’ is often hardly justified as interactions completely wash out Landau quasi-particles. The latter are ubiquitous in two and three dimensional Fermi systems \[20, 39\], and this provides the main theoretical justification for the use of mean-field theory in the calculation of band structures and other spectral properties of two- and three-dimensional systems. Indeed, it would be interesting to extend the type of studies reported here to higher dimensional systems. If our expectations are correct, the existence of stable Landau quasi-particles should make the predictions of mean-field theory for
the orbital current even more reliable. The difficulty in this case may be to find an unbiased method like DMRG to test the mean-field predictions against accurate numerical calculations of the orbital current and susceptibility. Experimentally, it would be interesting to measure the orbital current in an experiment like the one reported in reference [32], which studied a three-dimensional Fermi gas in a synthetic spin orbit field.

As far as one dimensional systems are concerned, this study has raised some issues that need to be addressed in more depth in future studies. One of them has been already pointed above, and concerns the investigation of interaction-induced gaps in the low energy sector and their impact on the behavior of the orbital current and susceptibility close to a Lifshitz transition. This may be especially relevant for systems with attractive interactions (e.g. for $U < 0$) since in this case the interaction and the inter-leg hopping favor different types of configurations in the ground state, and therefore compete with each other. For repulsive interactions a careful investigation of the system at half-filling (i.e. for $n = \frac{1}{2}$) is also necessary, as it has also been pointed out above. In addition, more accurate numerical studies using DMRG are required in order to understand the behavior of the entanglement entropy across the Lifshitz transition, and to assess to what extent the singularities exhibited by the orbital susceptibility are modified by the interaction effects. The latter study will require a careful finite-size analysis of the orbital current and susceptibility close to the transition.

Finally, in connection with recent [9, 10] and future experiments, finite temperature effects should be also considered. The extension of the mean-field theory developed here to finite temperatures is rather straightforward, but unbiased calculations of the orbital current or susceptibility at finite temperature using DMRG may be more demanding (although they have been already undertaken for the closely related system of interacting hard-core bosons in flux ladders [40]). Qualitatively, we expect that the quantum phase transitions of the Lifshitz type studied here will become crossovers, and finite temperature effects will round the sharpness of cusps in the orbital current and the singularities of the susceptibility.

Acknowledgments

The work of MT was partly supported by Grants-in-Aid No. JP17K17822, No. JP20H05270, No. JP20K03787, and No. JP21H05185 from MEXT of Japan. The work of MAC has been supported by Ikerbasque, Basque Foundation for Science and MICINN Grant No. PID2020-120614GB-I00 (ENACT). MAC thanks Masaki Tezuka and Norio Kawakami for their hospitality at Kyoto University during the final states of the completion of this manuscript.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Bloch-wave basis

In this appendix, we review the band structure of the system described by (1) in the non-interacting limit (i.e. for $U = 0$). In order to obtain the band dispersion, we follow [23] by applying the Fourier transform to the kinetic energy in equation (1),

$$
\epsilon_{q,\sigma} = \frac{1}{\sqrt{L}} \sum_{m} e^{i(q + \phi_{\sigma}) m} \epsilon_{m,\sigma},
$$

(A1)

followed by a unitary transformation in the ladder indices $\sigma$. In the above equation $\phi_{\sigma}$ is the phase for species (leg) $\sigma$. Setting $\phi_{\downarrow} = \phi_{\uparrow} = \phi$, the flux-dependence from the inter-leg hopping is eliminated, which renders the Hamiltonian to the following form:

$$
\hat{H}_0 = \sum_{q \in 1BZ,\sigma} \left[ -2t \cos(q + \phi_{\sigma}) c_{q,\sigma} \right] - \frac{\Omega}{2} \sum_{q \in 1BZ} \left( c_{q,\uparrow}^\dagger c_{q,\downarrow} + c_{q,\downarrow}^\dagger c_{q,\uparrow} \right),
$$

(A2)
where 1BZ corresponds to the segment \((-\pi, \pi]\) of lattice momenta in units where the lattice parameter \(a = 1\). The above Hamiltonian can be diagonalized by means of the following unitary transformation:

\[
\begin{pmatrix}
\epsilon_{\tilde{q}, u} \\
\epsilon_{\tilde{q}, d}
\end{pmatrix}
= \begin{pmatrix}
\cos \left[ \theta(q, \phi) \right] & \sin \left[ \theta(q, \phi) \right] \\
-\sin \left[ \theta(q, \phi) \right] & \cos \left[ \theta(q, \phi) \right]
\end{pmatrix}
\begin{pmatrix}
\epsilon_{q, u} \\
\epsilon_{q, d}
\end{pmatrix}.
\]

\(\text{(A3)}\)

Hence,

\[
\tilde{H}_0 = \sum_{q \in 1BZ} \left[ \epsilon_u(q, \phi) \tilde{c}_{q, u}^\dagger \tilde{c}_{q, u} + \epsilon_d(q, \phi) \tilde{c}_{q, d}^\dagger \tilde{c}_{q, d} \right],
\]

\(\text{(A4)}\)

where the single-particle dispersion \(\epsilon_s(q, \phi)\) is given by

\[
\epsilon_s(q, \phi) = -2t \cos \left( q + \frac{\phi_0 + \phi}{2} \right) \cos(\phi/2) \pm \frac{1}{2} \sqrt{\Omega^2 + \left[ 4t \sin \left( q + \frac{\phi_0 + \phi}{2} \right) \sin(\phi/2) \right]^2}.
\]

\(\text{(A5)}\)

The rotation angle of the unitary transformation can be obtained from the equation:

\[
\sin \left[ \theta(q, \phi) \right]^2 = \frac{1}{2} \left[ 1 - \frac{4t \sin \left( q + \frac{\phi_0 + \phi}{2} \right) \sin(\phi/2)}{\epsilon_u(q, \phi) - \epsilon_d(q, \phi)} \right],
\]

\(\text{(A6)}\)

and \(s = u, d\), where \(u \rightarrow +, (d \rightarrow -)\) stands for upper (lower) band. In figure 1, we show the band structure as a function of the flux \(\phi\) per plaquette and the ratio of hopping amplitudes, \(\Omega/t\). The red vertical line corresponds to the experimental situation considered in reference [9], which was carried out in the large \(\Omega/t\) regime. The band structure can be classified into four types according to whether there is band overlap between the upper and lower bands (cases A and B) or not (cases C and D), and whether the curvature of the lower band at \(q = 0\) is positive (A and D) or negative (B and C, cf figure 1). Note that, whenever there is no band overlap as it is the case for sufficiently large \(\Omega/t\) the lower band curvature determines whether only two Fermi points can exist (positive curvature at \(q = 0\)) or four Fermi points can exist for certain band filling (negative curvature at \(q = 0\)).

Next, we briefly consider the effects of the interaction in the basis of Bloch states. In this basis the inter-species (inter-leg) interaction takes the form:

\[
\tilde{U} = \frac{1}{U} \sum_{p,q} \tilde{U}(p, k; q; \phi) \tilde{c}_{p, u}^\dagger \tilde{c}_{q, u} \tilde{c}_{q-k, u}^\dagger \tilde{c}_{p+k, u} + \tilde{U}',
\]

\(\text{(A7)}\)

where \(\tilde{U}'\) involves the creation and destruction operators in the upper band. In the above expression:

\[
\tilde{U}(p, k; q; \phi) = U \Gamma(p, k, \phi) \Gamma(p + q, k - q, \phi),
\]

\(\text{(A8)}\)

\[
\Gamma(p, k, \phi) = \frac{1}{2} \left\{ \sin \left[ \theta(p, \phi) \right] \cos \left[ \theta(k, \phi) \right] - \sin \left[ \theta(k, \phi) \right] \cos \left[ \theta(p, \phi) \right] \right\}.
\]

\(\text{(A9)}\)

In the regime of interest in this work where \(\Omega \gtrsim 4t\), there is a large gap \(\sim \Omega\) between the lower and upper bands. Therefore, at low temperatures and for weak interactions (i.e. \(\tilde{U} \ll \Omega\)) and low filling (\(n \ll 1\)), it is safe to neglect scattering processes involving states in the upper band described by \(\tilde{U}'\) in equation (A7). In this regard, we note that, for small \(\phi\), \(\Gamma(p, k, \phi = 0) \sim \phi^2\), which means that, for \(2t/\Omega \ll 1\) and \(\tilde{U} \ll \Omega\), the (inter-leg) interaction has a rather weak effect on the system, as it has been already discussed in section 4.1 by working in a different basis. Indeed, in the limit where \(2t/\Omega \ll 1\), we have

\[
\tilde{U} = U \left( \frac{2t}{\Omega} \right)^2 \sin^2(\phi/2) \cos^2(Q) \sin(q_1) \sin(q_2) + O \left( \frac{2t}{\Omega} \right)^4,
\]

\(\text{(A10)}\)

where \(Q = (p + k)/2\), and \(q_1 = (k - p)/2, q_2 = (k - p - 2q)/2\). This expression makes it clear that the effect of the interactions is suppressed by powers of \((t/\Omega)^2 \ll 1\) in the large \(\Omega\) limit. Note as well that for \(U \gtrsim \Omega\) and \(\phi \sim \pi\), the effect of the interaction becomes more important.

A1. Perturbation theory

In the weakly interacting case (i.e. for \(4U \tilde{t}^2 \sin^2(\phi)/\Omega^3 \ll 1\)), the chemical potential can be approximately determined using non-interacting model since the chemical potential is of order \(-\Omega/2\) and is much larger
than the Hartree–Fock shift $\sim 4Ut^2 \sin^2(\phi)/\Omega^2$. From equation (25), the orbital current can be calculated from the effective Hamiltonian:

$$J(N, \phi) = -\sum_{\sigma=\uparrow,\downarrow} \sum_q \frac{\partial c_{\sigma q}(\phi)}{\partial \phi} n_{\sigma q}(\phi) - \sum_{p, k, q} \frac{\partial \tilde{U}(p, k, \mu; \phi)}{\partial \phi} \langle \hat{c}_{p \sigma q} \hat{c}_{k \sigma \mu q} \hat{c}_{k \downarrow p \mu q} \rangle .$$  \hspace{1cm} (A11)

Hence, the orbital susceptibility can be obtained as $\chi = L^{-1} \partial f/\partial \phi$.

The leading order contribution to the orbital current stems from the interaction term since the first-order correction to momentum distribution vanishes. This is nothing but the derivative of the Hartree–Fock correction to the total energy:

$$f^{(1)} = \frac{1}{L} \sum_{p, k, q} \frac{\partial \tilde{U}(p, k, \mu; \phi)}{\partial \phi} \langle \hat{c}_{p \sigma q} \hat{c}_{k \sigma \mu q} \hat{c}_{k \downarrow p \mu q} \rangle = \frac{2U}{L} \sum_{p, k} \frac{\partial \Gamma(p, k; \phi)}{\partial \phi} n_{d \sigma p} n_{d \downarrow k},$$  \hspace{1cm} (A12)

where $n_{d \sigma p}$ stands for the non-interacting Fermi–Dirac distribution. The total orbital current including the Hartree–Fock correction is shown on the left panel of figure 8. We note the leading order correction suffices to qualitatively capture the interaction-induced change from diamagnetic to paramagnetic behavior at small $\phi$ in the regime where $4Ut^2 \sin^2(\phi/2)/\Omega^2 \ll 1$.

Appendix B. Results for non-interacting fermions

B1. Orbital current at fixed particle number

In this appendix, we review the most important results for the orbital current in the absence of interactions. As explained in section 3, the orbital current can be calculated from the partition function, which for the non-interacting system is:

$$Z_0 = \prod_{s=u,d} \prod_q \left[ 1 + e^{-\beta E_{q}(s)} + \beta \mu(s) \right] .$$  \hspace{1cm} (B1)

Hence, the free energy for fixed particle number is obtained:

$$G^{(0)}(N, \phi) = -\frac{1}{\beta} \log(Z_0) + N\mu(\phi).$$  \hspace{1cm} (B2)

Thus, the orbital current is:

$$f^{(0)}(N, \phi) = -\frac{\partial}{\partial \phi} G^{(0)}(N, \phi) = -\sum_{s=u,d} \sum_q n_{q\sigma}(0) \frac{\partial \epsilon_{q\sigma}(\phi)}{\partial \phi},$$  \hspace{1cm} (B3)

where $n_{q\sigma}^{(0)}$ is the Fermi distribution function. Figure 3 shows the results of evaluating this expression for the orbital current density $f^{(0)}(N, \phi)/L$ at zero temperature for several values of the lattice filling $n = N/L$. We note that there are two non-trivial features in the behavior of current: (1) at large lattice filling and small orbital current density $\phi$, the sign of the orbital current is the opposite (negative in our convention) to the sign at low lattice fillings.

And (2) near the sign of the orbital current is the opposite (negative in our convention) to the sign at low lattice fillings.

B2. Orbital susceptibility near $\phi = 0$

Next, we study the zero-field orbital susceptibility defined as $\chi_0 = L^{-1} \langle \partial f/\partial \phi \rangle_{\phi=0}$. For $\chi_0 > 0$ ($\chi_0 < 0$) we speak of paramagnetic (diamagnetic) behavior of the orbital current is induced by the gauge field. At low temperatures where only the lower band is occupied, we obtain:

$$\chi_0 = -\frac{2}{2\pi} \int_0^{\rho_0} \frac{t}{t} \left[ \cos(q) - \frac{4t \sin^2(q)}{\Omega} \right] dq = -\frac{t}{2\pi} \left[ \sin(n\pi) + \frac{t(\sin(2n\pi) - 2n\pi)}{\Omega} \right].$$  \hspace{1cm} (B4)

In the last line, we have used that $n = k_0^0 / \pi$. The boundary for the transition from paramagnetic to diamagnetic behavior is obtained by solving the following equation:

$$\frac{t}{2\pi} \left[ \sin(n\pi) + \frac{t(\sin(2n\pi) - 2n\pi)}{\Omega} \right] = 0,$$  \hspace{1cm} (B5)
for the hopping strength ratio $\Omega/t$ and the particle density $n$. Figure 3 shows this boundary between the diamagnetic and paramagnetic behavior obtained in this fashion.

### Appendix C. Orbital susceptibility near Lifshitz transitions for non-interacting fermions

In this appendix, we obtain a number of exact expressions for the energy density, orbital current and susceptibility in the thermodynamic limit for the non-interacting system at zero temperature. We consider two different types of constraints: fixed chemical potential and fixed particle number.

#### C1. Thermodynamic limit

In the large $\Omega$ limit of interest in this work and at zero temperature, it is safe to neglect the contribution from the upper band. Therefore, the following expression for energy density in thermodynamic limit can be obtained:

$$\epsilon(\phi) = \int_{1BZ} \frac{dq}{2\pi} n_{q,\phi} \epsilon(q, \phi) = \frac{2}{2\pi} \int_{k_{F1}(\phi)}^{k_{F2}(\phi)} \epsilon(q, \phi) dq,$$

where $0 < k_{F1}(\phi) < k_{F2}(\phi)$ are the Fermi momenta in the four Fermi-point phase. In the case of the two Fermi-point phase, we should take $k_{F1}(\phi) = 0$. Finally, for the insulator phase for which the number of Fermi points is zero, $k_{F1}(\phi) = 0, k_{F2}(\phi) = \pi$. The values of the Fermi momenta are obtained below for both fixed chemical potential and fixed particle number. In the above expression, we have also introduced the notation $f(k_f)^2 = f(k_{F2}) - f(k_{F1})$ for a given function $f(k_f)$. A closed form for the function $\tilde{\epsilon}(\phi, k_f)$ in equation (C3) can be given in terms of the incomplete elliptic integral of the second kind:

$$E(k_f, m) = \int_{0}^{k_f} \sqrt{1 - m \sin^2 \theta} \, d\theta.$$  

Hence, the energy density can be obtained from the following expression:

$$\tilde{\epsilon}(\phi, k_f) = -2t \cos(\phi/2) \sin(k_f) - \Omega \frac{1}{2} E(k_f, -g^2),$$

where $g = 4t \sin(\phi/2)/\Omega$. Thus, the orbital current density at fixed chemical potential is

$$J_{\mu} = -\frac{1}{\beta} \frac{\partial G(\beta, \mu, \phi)}{\partial \phi} = \frac{1}{L} \left\langle \left( \frac{\partial H}{\partial \phi} - \mu \frac{\partial N}{\partial \phi} \right) \right\rangle,$$

where $G(\beta, \mu, \phi)$ is the thermodynamic potential. For fixed number of particles, it is

$$J_{n} = -\frac{1}{\beta} \frac{\partial}{\partial \phi} \left[ G(\beta, \mu, \phi)/L + n \mu \right] = \frac{1}{L} \left\langle \frac{\partial H}{\partial \phi} \right\rangle.$$

As explained in section 2, at zero temperature the orbital current with fixed particle number and chemical potential are given by

$$J_{o}(\phi) = \frac{1}{\pi} \frac{\partial \tilde{\epsilon}(\phi, k_f(\phi))}{\partial \phi} |_{1}^{2} = \frac{1}{\pi} \tilde{J}(\phi, k_f(\phi)) |_{1}^{2},$$

$$J_{\mu}(\phi) = J_{o}(\phi) - \mu \left( \frac{\partial n(\phi)}{\partial \phi} \right).$$

From these expressions and in the limit of large $\Omega$, we can derive the orbital current density using the following relations for the elliptic integral function:

$$\frac{\partial E(k, m)}{\partial k} = \sqrt{1 - m \sin^2(k)},$$

$$\frac{\partial E(k, m)}{\partial m} = \frac{E(k, m) - F(k, m)}{2m}.$$
where $F(k, m)$ is the incomplete elliptic integral of the first kind:

$$F(k, m) = \int_0^k \frac{1}{\sqrt{1 - m \sin^2 \theta}} \, d\theta.$$  \hfill (C12)

Hence,

$$\tilde{J}(\phi, k_F) = \frac{1}{\pi} \frac{\partial k_F}{\partial \phi} \epsilon(\phi, k_F) + t \sin(\phi/2) \sin(k_F) - \Omega \cot(\phi/2) \frac{E(k_F, g^2) - F(k_F, g^2)}{4}. \hfill (C13)$$

We note that, for fixed chemical potential, the first term on right hand-side of the above expression is exactly cancelled by the second term in equation (C9) since $\epsilon(k_F, \phi) = \mu$.

The susceptibility is obtained from the derivative of orbital current using the following identities:

$$\frac{\partial F(k, m)}{\partial k} = -\frac{1}{\sqrt{1 - m \sin^2(k)}}, \hfill (C14)$$

$$\frac{\partial F(k, m)}{\partial m} = -\frac{E(k, m) + (m-1)F(k, m)}{2m(m-1)} \frac{\sin(2k)}{4(m-1)\sqrt{1 - m \sin^2(k)}}. \hfill (C15)$$

Applying the derivatives to $\tilde{\epsilon}$ yields:

$$\chi_\alpha(\phi) = \frac{1}{\pi} \tilde{\chi}(\phi, k_F)^2_\alpha, \hfill (C16)$$

$$\chi_\mu(\phi) = \frac{1}{\pi} \tilde{\chi}(\phi, k_F)^2_\mu - \frac{\partial^2 n(\phi)}{\partial \phi^2} \mu, \hfill (C17)$$

where we have introduced the following function

$$\tilde{\chi}(\phi, k_F) = \left[ \frac{\partial^2}{\partial \phi^2} + 2 \frac{\partial k_F}{\partial \phi} \frac{\partial}{\partial k_F} + \frac{\partial^2 k_F}{\partial \phi^2} \frac{\partial}{\partial k_F} + \left( \frac{\partial k_F}{\partial \phi} \right)^2 \frac{\partial}{\partial k_F} \right] \tilde{\epsilon}(\phi, k_F),$$

$$= \frac{1}{\pi} \left[ 2 \frac{\partial k_F}{\partial \phi} \frac{\partial}{\partial \phi} + \frac{\partial^2 k_F}{\partial \phi^2} \frac{\partial}{\partial k_F} + \left( \frac{\partial k_F}{\partial \phi} \right)^2 \frac{\partial}{\partial k_F} \right] \epsilon(\phi, k_F) + \frac{1}{\pi} \frac{\partial^2 \epsilon(\phi, k_F)}{\partial \phi^2}. \hfill (C18)$$

In the second equation we have used $\partial_{k_F} \tilde{\epsilon}(\phi, k_F) = \epsilon_d(\phi, k_F)$, i.e. the dispersion relation of the lower band. Note that the last term involves a partial derivative with respect to $\phi$ and it can be also written as:

$$\frac{1}{\pi} \frac{\partial^2 \tilde{\epsilon}(\phi, k_F)}{\partial \phi^2} = \int_0^{k_F} \frac{dq}{\pi} \frac{\partial^2 \epsilon_d(q, \phi)}{\partial \phi^2}. \hfill (C19)$$

The above function after setting $k_F = k_{F1,2}(\phi)$ is a continuous function of $\phi$. In the following section, we shall see that the Fermi momenta $k_{F1,2}(\phi)$ are continuous functions of $\phi$, but their derivatives are not. Thus, any possible singularities in the orbital susceptibility must arise from the terms in equation (C18) that contain derivatives of the Fermi momenta with respect to $\phi$. In connection to this, it is important to note that, in the case of fixed particle density, the susceptibility depends on the first and second order derivatives of the Fermi momenta with respect to $\phi$. However, for fixed chemical potential, using equations (C17) and (C18), the second order derivative of $k_F$ with respect to $\phi$ is cancelled and the orbital susceptibility only depends on the first derivative.

**C2. Numerical determination of the Fermi points**

For fixed chemical potential, the location Fermi momenta can be obtained from

$$\epsilon_d(q, \phi) = \mu, \hfill (C20)$$
Figure 13. Largest Fermi momentum, $k_{F2}$, and its derivatives as a function of $\phi$ for two types of constraints (fixed lattice filling $n$ and fixed chemical potential $\mu$). We note that, for fixed $\mu$, the Fermi momentum exhibits a square root dependence which gives rise to a $(\phi - \phi_c)^{-1/2}$ singularity in $\partial k_{F}/\partial \phi$. This is characteristic of a van Hove singularities in one dimension. The second derivative $\propto \partial^2 k_{F}/\partial \phi^2$ is cancelled (cf equation (C18) and following). For fixed particle number, the dependence of the Fermi momentum on $\phi$ gives rise a delta-function. (Resulting from $\partial^2 k_{F}/\partial \phi^2$ singularity in the susceptibility at the transition point and a step-function (resulting from $\propto \partial k_{F}/\partial \phi$) behavior near the transition point.

which can be solved analytically. For fixed particle number, the Fermi points are related by the relation:

$$n = \frac{N}{L} = \int_{k_{F1}(\phi)}^{k_{F2}(\phi)} \frac{dq}{\pi} = k_{F2}(\phi) - k_{F1}(\phi). \quad (C21)$$

This relation determines only one of the Fermi points. The other can be obtained by requiring that

$$\epsilon_d(k_{F1}(\phi), \phi) = \epsilon_d(k_{F2}(\phi), \phi) + \epsilon_d(k_{F1}(\phi) + \pi n, \phi). \quad (C22)$$

Note that in the two Fermi-point phase, we must set $k_{F1} = 0$. In the four Fermi-point phase where $k_{F1}, k_{F2} \neq 0$, the above equation can be solved numerically to high precision.

Figure 13 shows the behavior of the (largest) Fermi momentum numerically obtained for $n = 0.75$ and fixed chemical potential ($\mu = -0.372t$). On the same figure, we also show the first and second derivatives of the Fermi momentum. For fixed chemical potential, the first derivative exhibits square root dependence with the magnetic flux. However, for fixed particle number, the first order derivative is a step function whereas the second order derivative contains both a step discontinuity and a Dirac delta-function singularity (resulting from the discontinuity of the first derivative) at the critical point [41]. Using these results along with equation (C18), we will next investigate the singularities of the orbital susceptibility near the critical point.

C3. Singular behavior of the orbital susceptibility

Using the previous results, we have obtained the critical behavior of the orbital susceptibility for fixed chemical potential and fixed particle number. Plots of the susceptibility for fixed particle number and fixed
chemical potential are shown in figures 2 and 14. The results of figure 2 are obtained for a finite system for which the singularities in the orbital current and susceptibility are slightly broadened by the finite-size effects. To investigate the singular behavior, we have plotted in figure 14 the same quantity in the thermodynamic limit as obtained from the above formulas and focused on the regime near the critical point of the Lifshitz transition. For fixed $\mu = -0.732t$ (lower panel of figure 14), an inverse square-root divergence $\sim(\phi - \phi_c)^{-1/2}$ is observed. In this case, the system undergoes a transition between a metal with two Fermi points and a band insulator. The same critical behavior is observed at another choice of fixed $\mu = -2.5t$, which is shown on figure 15. In the latter case, the Lifshitz transition takes place by changing the number of Fermi points changing between two and four. These results demonstrate that the singular behavior at the critical point is determined by the constraint of fixed chemical potential. The inverse square-root singularity arises from the van Hove singularity in the density of states at the top of the lower band because, as $\phi$ is varied, the top of the lower band must cross the Fermi level. Using the results obtained in the previous subsection, we can see that the inverse square-root singularity stems from the same singularity displayed by $\partial\phi k_F(\phi)$ (cf figure 13).
Finally, let us consider the case of fixed particle number. Using equation (C18) shows that \( \chi_n \) we see that \( \chi_n \) depends both of the first and second derivative of the Fermi momentum. For this constraint, the Fermi momentum close to the Lifshitz transition \( k_{F2}(\phi) \) grows from a constant value approximately linearly (cf figure 13). \( k_{F1}(\phi) \) is continuous, but its first and second derivatives, upon which \( \chi_n \) depends, exhibit a step-like discontinuities and a Dirac-delta singularity, which can be also seen on figure 14 (lower panel) and figure 2 (right panel) for \( \chi_n \).

### Appendix D. Mean-field theory

The mean-field Hamiltonian in equation (41) can be solved numerically on a finite lattice by exact diagonalization, which allows us to self-consistently determine the mean-field parameters. Let us introduce a vector notation where \( \mathbf{u}^\dagger \) is given by

\[
\mathbf{u}^\dagger = \left\{ c_{\uparrow,1}^\dagger, c_{\downarrow,1}^\dagger, c_{\uparrow,2}^\dagger, c_{\downarrow,2}^\dagger, \ldots, c_{\uparrow,L}^\dagger, c_{\downarrow,L}^\dagger \right\}. \tag{D1}
\]

Thus, the mean-field Hamiltonian can be written as follows:

\[
\hat{H}^{MF} = \mathbf{u}^\dagger \hat{H}^{MF} \mathbf{u}. \tag{D2}
\]

Let \( \{ |\nu_i\rangle = |\nu_{i,\uparrow}, |\nu_{i,\downarrow}, \ldots, |\nu_{i,L,\uparrow}, |\nu_{i,L,\downarrow} \rangle \} \) be the eigenvectors of the mean-field Hamiltonian matrix \( \hat{H}^{MF} \) with eigenvalues \( \{ \epsilon_i \} \), i.e.

\[
\hat{H}^{MF} |\nu_i\rangle = \epsilon_i |\nu_i\rangle. \tag{D3}
\]

Hence, the mean-field parameters can be obtained from the following expressions:

\[
\alpha_m(\phi) = \sum_{\langle ij \rangle} (\nu_{me}^j)^\ast \nu_{mj}^i, \tag{D4}
\]

\[
n_{m,\uparrow} = \sum_{\langle ij \rangle} (\nu_{me}^i)^\ast \nu_{mj}^i, \tag{D5}
\]

\[
n_{m,\downarrow} = \sum_{\langle ij \rangle} (\nu_{me}^i)^\ast \nu_{mj}^i. \tag{D6}
\]

The latter are a set of equations that need to be solved self-consistently since the coefficients \( \nu_{me}^i \) depend on the mean-field parameters themselves. Note that in the above equations we have used the notation \( \sum_{\langle ij \rangle} \), which means that the summation is over the lowest \( N = L \times n \) eigenstates for \( N \) particles. From the self-consistent solution, e.g. the total orbital current on the \( \sigma = \uparrow \)-leg can be computed as follows:

\[
J_{\uparrow}^{MF} = 2 \text{Im} \left[ \sum_m \sum_{\langle ij \rangle} (\nu_{me}^i)^\ast \nu_{mj+1,\uparrow} e^{i\phi/2} \right] = \sum_m j_{m,\uparrow}, \tag{D7}
\]

where \( j_{m,\uparrow} \) is the local orbital current.

### Appendix E. Convergence of the DMRG results

Figure 16 shows the DMRG results for the orbital current for different system sizes and number of block states and interaction strength \( U/t = 0, 5 \) compared to the analytical result obtained in thermodynamic limit (see appendix C1) for the non-interacting case. The weak dependence on the system size \( L \) and the number of block states \( m \) indicates that our numerical results can be trusted for discussing the thermodynamic limit of the system.
Figure 16. Convergence of the DMRG results for the orbital current. We used $\Omega/t = 4.28$, $n = 0.75$, $U/t = 0$ and $U/t = 5$. We computed two different system sizes, $L = 64, 128$, and used two values of the DMRG block size $m = 128, 192$. The dashed line for the non-interacting case corresponds to the analytical result in the thermodynamic limit. The DMRG result for $L = 128, m = 192$ deviates from the analytical result by less than $1\%$ for most points (the relative deviation becomes larger when the magnitude of the orbital becomes very small). For the interacting case, the difference between $L = 128, m = 128$ and $L = 128, m = 192$ is within the point size.

ORCID iDs

Masaki Tezuka  
https://orcid.org/0000-0001-7877-0839

Miguel A Cazalilla  
https://orcid.org/0000-0002-2994-2873

References

[1] Cooper N R, Dalibard J and Spielman I B 2019 Rev. Mod. Phys. 91 015005
[2] Aidelsburger M, Lohse M, Schweizer C, Atala M, Barreiro J T, Nascimbène S, Cooper N R, Bloch I and Goldman N 2014 Nat. Phys. 11 162
[3] Aidelsburger M, Atala M, Lohse M, Barreiro J T, Paredes B and Bloch I 2013 Phys. Rev. Lett. 111 185301
[4] Miyake H, Siviloglou G A, Kennedy C J, Burton W C and Ketterle W 2013 Phys. Rev. Lett. 111 185302
[5] Strinati M C, Cornfeld E, Rossini D, Barbarino S, Dalmonte M, Fazio R, Sela E and Mazza L 2017 Phys. Rev. X 7 021033
[6] Cornfeld E and Sela E 2015 Phys. Rev. B 92 115146
[7] Wauters M and Santoro G E 2018 Phys. Rev. B 98 205112
[8] Wall M L, Koller A P, Li S, Zhang X, Cooper N R, Ye J and Rey A M 2016 Phys. Rev. Lett. 116 035301
[9] Livi L et al 2016 Phys. Rev. Lett. 117 220401
[10] Mancini M et al 2015 Science 349 1510
[11] Barbarino S, Taddia L, Rossini D, Mazza L and Fazio R 2016 New J. Phys. 18 035010
[12] Taddia L, Cornfeld E, Rossini D, Mazza L, Sela E and Fazio R 2017 Phys. Rev. Lett. 118 230402
[13] Chen G, Hazzard K R A, Rey A M and Hermele M 2016 Phys. Rev. A 93 061601
[14] Stenzel L, Hayward A L C, Schollwöck U and Heidrich-Meisner F 2020 Phys. Rev. A 102 023315
[15] Haller A, Rizzi M and Burrello M 2018 New J. Phys. 20 053007
[16] Haller A, Rizzi M and Filippone M 2020 Phys. Rev. Res. 2 023058
[17] Stuhl B K, Lu H-I, Aycock L M, Genkina D and Spielman I B 2015 Science 349 1514
[18] Celi A, Massignan P, Ruseckas J, Goldman N, Spielman I B, Juzeliūnas G and Lewenstein M 2014 Phys. Rev. Lett. 112 043001
[19] An F A, Meier E J and Gadway B 2017 Sci. Adv. 3 e1602685
[20] Giamarchi T 2003 Quantum Physics in One Dimension (International Series of Monographs on Physics) (Oxford: Clarendon)
[21] Buer M, Greschner S, Schollwöck U and Giamarchi T 2021 Phys. Rev. Lett. 126 030501
[22] Carr S T, Narovchyn B N and Nersesyan A A 2006 Phys. Rev. B 73 195114
[23] Roux G, Orignac E, White S R and Poullblanc D 2007 Phys. Rev. B 76 195105
[24] White S R 1992 Phys. Rev. Lett. 69 2863
[25] White S R 1993 Phys. Rev. B 48 10345
[26] Schollwöck U 2005 Rev. Mod. Phys. 77 259–315
[27] Hallberg K A 2006 Adv. Phys. 55 477–526
[28] Benilagia A and Vojta M 2013 Phys. Rev. B 87 165143
[29] Ptok A, Kapcia K J, Cichy A, Oleś A M and Piekarz P 2017 Sci. Rep. 7 41979
[30] Wu S, Zhang Z, Watanabe K, Taniguchi T and Andrei E Y 2021 Nat. Mater. 20 488
[31] Volovik G E 2017 Low Temp. Phys. 43 47
[32] Wang P, Yu Z-Q, Fu Z, Miao J, Huang L, Chai S, Zhai H and Zhang J 2012 Phys. Rev. Lett. 109 095301
[33] Bauer B et al 2011 J. Stat. Mech. P05001
[34] Albuquerque A F et al 2017 J. Magn. Magn. Mater. 310 1187
[35] Sun G, Jaramillo J, Santos L and Vekua T 2013 Phys. Rev. B 88 165101
[36] Huang C-H, Tezuka M and Cazalilla M A (in preparation)
[37] Rodney M, Song H F, Lee S-S, Le Har K and Sørensen E S 2013 Phys. Rev. B 87 115132
[38] Cazalilla M A 2004 J. Phys. B: At. Mol. Opt. Phys. 37 S1
[39] Baym G and Pethick C 2008 Landau Fermi-Liquid Theory: Concepts and Applications (New York: Wiley)
[40] Buser M, Hubig C, Schollwöck U, Tarruell L and Heidrich-Meisner F 2020 Phys. Rev. A 102 053314
[41] This result can be obtained analytically if we solve equation (C23) using a ‘toy model’ dispersion $\epsilon(k, \phi) = a(\phi) - (\phi - \phi_0)$

$$k^2/2m + \lambda k^4/4, \text{ with } a(\phi), m, \lambda > 0.$$ This dispersion has the same ‘double well’ structure as the lower band dispersion for $\phi > \phi_0$. 