The recent discovery of materials featuring strong Rashba spin-orbit coupling (RSOC) and strong electronic correlation raises questions about the interplay of Mott and Rashba physics. In this work, we employ cluster perturbation theory to investigate the spectral properties of the two-dimensional Hubbard model in the presence of a significant or large RSOC. We show that RSOC strongly favors metallic phases and competes with Mott localization, leading to an unconventional scenario for the Mott transition which is no longer controlled by the ratio between the Hubbard $U$ and an effective bandwidth. The results show a strong sensitivity to the value of the RSOC.

The breaking of inversion symmetry has important consequences on the properties of matter. Just to mention a few examples, inversion symmetry breaking yields unconventional superconducting pairing [1] [35], it controls magnetic ordering at interfaces and surfaces [2], it rules the generation of spin currents [3] [36], and it determines the locking of spin and quasi-momentum in Rashba metals [6] [7]. Furthermore, inversion symmetry breaking effects can be controlled and enhanced by material engineering [8] [13] and gating [14] [15]. In a large class of materials and heterostructures [10] [12] [13] [16], inversion symmetry breaking effects coexist with electron-electron correlation. This calls for a systematic study of the interplay between these two effects, which, on one hand, will help us to understand parity-violating phenomena in actual solids where interactions are significant and on the other, owing to the intrinsic tendency of correlated systems towards magnetic ordering, holds a huge potential for the development of antiferromagnetic spintronics [17] [18].

Motivated by these findings, in the present work we focus on a well-known consequence of inversion symmetry breaking, namely, Rashba spin-orbit coupling (RSOC) [19], and we show that it significantly affects Mott physics and correlation induced localization effects. Various works describing the interplay of RSOC and electronic correlation were mainly focused on the structure of the phase diagram [20], on the investigation of topological effects [21] [22] and on the properties of the associated Fermi liquid [23] [24].

In this work we focus on the fundamental question of how the presence of RSOC modifies the correlation-driven Mott transition and on the characterization of the spectral signatures of electronic correlation in materials with strong RSOC. In Ref. [25] we showed that in small Hubbard clusters the presence of RSOC contrasts the localization effect of the interaction and favors a metallic ground-state through a mixing between singlet and triplet components which enables a new screening mechanism of local interactions. We called this new metallic state Pauli metal. Here, we consider the two-dimensional Hubbard model on a square lattice and we investigate its spectral properties in the presence of RSOC. We show that RSOC counteracts localization effects, yielding qualitative and quantitative modifications in the Mott transition and favoring the onset of a metallic phase. Depending on the strength of Hubbard repulsion the latter may be very different from the standard weakly interacting Rashba Fermi liquid. In particular, we show that, due to the strong momentum dependence of the spectral weights of the two Hubbard bands, a pseudogap phase appears at the transition between the Rashba metal and the Mott insulator. Our work thus demonstrates a non-trivial interplay between Mott physics and RSOC hinting at an enhancement of transport in strongly correlated systems in the presence of RSOC, opposite to what happens in weakly interacting disordered Fermi gases [26] [28]. This result may be extremely relevant to account for the transport properties of oxides heterostructures [29], surface alloys [10] and polar semiconductors [13] [19] [30].

We consider the following Rashba-Hubbard model:

$$H = H_0 + H_U.$$  \hfill\( (1)\)

where $H_U$ is the Hubbard interaction,

$$H_U = U \sum_i n_{i\uparrow} n_{i\downarrow},$$  \hfill\( (2)\)

while $H_0$ can be written as the sum of a standard spin-diagonal hopping and a spin-flip Rashba hopping term.
between nearest-neighboring sites as follows
\[ H_0 = -t \sum_{\langle ij \rangle} c^\dagger_i c_j - t_R \sum_{\langle ij \rangle} c^\dagger_i (\vec{\alpha}_{ij} \times \vec{\sigma})_z c_j \] (3)
where we introduced the local spinor creation and annihilation operators \( c^\dagger_i \) and \( c_i \) and we defined the vector \( \vec{\alpha}_{ij} = (\alpha_{ij}^x, \alpha_{ij}^y) \) with \( \alpha_{ij}^\mu = i(\delta_{ij+a_\mu} - \delta_{ij-a_\mu}) \) where \( a_\mu \) is the unitary translation in the \( \mu \) direction.

To properly describe the competition of \( H_0 \), with its inherently non-local nature, and \( H_U \), we use cluster perturbation theory \([31, 32]\) (CPT). We thus divide the lattice into a superlattice of identical clusters and we calculate the electronic Green’s function, \( G(\omega, \mathbf{k}) \), treating the inter-plaquette hopping perturbatively. In this work we choose a four-site plaquette which, as stressed in Ref.\([25]\), is the minimal cluster where the non-abelian gauge structure of Rashba coupling can emerge. With this choice, our study encompasses the Pauli screening mechanism discussed in Ref.\([25]\) and preserves the basic symmetries of the lattice.

We tile the lattice as shown in Fig. 1 and we decompose the lattice vectors as \( \mathbf{r}_i = \mathbf{r}_m + \mathbf{r}_a \) where \( \mathbf{r}_a \) refers to the position of the lowermost left site of each plaquette while \( \mathbf{r}_a \) indicates the position of the site in the plaquette. To have uniform spin-rotations upon tunneling along \( x \) and \( y \) in the lattice, we set RSOC with opposite signs on adjacent plaquettes. The Hamiltonian is in turn partitioned as follows:
\[ H = H_{\text{loc}} + V \] (4)
where \( H_{\text{loc}} \) contains all the intra-cluster terms (diagonal in the index \( m \)) including interaction while \( V \) accounts for the inter-plaquette hopping.

Following the route suggested e.g. in Ref.\([32]\), we perform a partial Fourier transformation with respect to the cluster position indices describing the Hamiltonian \( H \) in the mixed representation. In this representation \( V \) can be recast as follows
\[ V = -\sum_{k,a,b} c^\dagger_{ak} \tilde{T}_{ab}(\mathbf{k}) c_{bk}. \] (5)
where \( k \) belongs to the Brillouin zone of the original lattice while the inter-plaquette hopping amplitude \( \tilde{T}_{ab}(\mathbf{k}) \) is represented by a \( 2 \times 2 \) matrix spin space. The full inter-plaquette hopping matrix has thus dimension 8 and it can be written as follows
\[
\tilde{T}(\mathbf{k}) = (e^{-2ik_x(\tau_0 + it_R\sigma_0)} \otimes \tau_x + e^{-2ik_y(\tau_0 - it_R\sigma_0)} \otimes \tau_y + \text{H.c.})
\] (6)
with the matrices \( \tau_x \) and \( \tau_y \) denoting forward unitary translations in the \( x \) and \( y \) direction in the plaquette. Starting from Eqs.\([40]\) we obtain the following expression for the Green’s function of the lattice
\[ G(\omega, \mathbf{k}) = \frac{1}{4} \sum_{a,b} \tilde{g}_{ab}(\omega, \mathbf{k}) e^{i\mathbf{k}(\mathbf{r}_a - \mathbf{r}_b)} \] (7)
where \( a \) and \( b \) enumerate the sites in the plaquette and \( \tilde{g}_{ab}(\omega, \mathbf{k}) \) is a \( 2 \times 2 \) matrix in spin-space denoting the single-particle Green’s function of \( H \) to lowest order in the inter-plaquette hopping \( V \) \([33]\) i.e.
\[ \tilde{g}(\omega, \mathbf{k}) = \left[ \tilde{g}_{\text{loc}}^{-1}(\omega) - \tilde{T}(\mathbf{k}) \right]^{-1} \] (8)
where \( \tilde{g}_{\text{loc}}(\omega) \) is the exact plaquette’s Green’s function. The overall structure of the spectrum can be then deduced from the spectral function, \( A_0(\omega, \mathbf{k}) \), defined as
\[ A_0(\omega, \mathbf{k}) = -\frac{1}{\pi} \text{Im} \text{Tr} [G(\omega, \mathbf{k})] \] while the spin-polarization of the states can be described using the spin-projected spectral function \( A_\mu(\omega, \mathbf{k}) = -\frac{1}{\pi} \text{Im} \text{Tr} [G(\omega, \mathbf{k})\sigma_\mu] \) with \( \mu = x, y, z \).

We first discuss the standard strong coupling regime, \( U \gg t \gg t_R \), where the system is in a Mott insulating phase and we can use a standard strong-coupling expansion to obtain renormalized eigenvalues of the system. Within this approximation the self-energy is independent of spin and momentum and the interacting spectrum consists of four bands with dispersion
\[ \xi_{kl\nu} = \frac{U + E_{kl} + \nu \sqrt{U^2 + E_{kl}^2}}{2} \] (9)
where the index \( \nu = \pm \) identifies the upper and lower
FIG. 3: Evolution of the spectrum across the Mott transition along the axis $k_x$, red and blue colors indicate positive and negative $y$-polarization. Mott insulating phases for weak and strong spin-orbit are shown on the upper and lower leftmost panels while metallic phases for, respectively, strong and weak interaction are shown on the rightmost panels. Specifically, upper panels, (a-e), show $A_y(\omega, k)$ for $t_R \in [0, 2t]$ and $U = 6t$ while lower panels, (f-j), show $A_y(\omega, k)$ for $t_R = 2t$ and $U \in [16t, 2t]$.

Hubbard band while the index $\lambda = \pm$ indicates the helicity with $E_{kl\lambda}$ denoting the dispersion of the helical bands in the absence of interaction,

$$E_{kl\lambda} = \epsilon_0(k) + 2\lambda t_R \sqrt{\sin^2 k_x + \sin^2 k_y},$$

where we defined $\epsilon_0(k) = -2t \left[ \cos(k_x) + \cos(k_y) \right]$ and we set $a_x = a_y = 1$.

As shown in Fig. 2(a-b) where we compare the CPT spectral function, $A_0(\omega, k)$ to that obtained using the strong-coupling approximation, $A_{0c}(\omega, k)$, the latter yields a good qualitative description of the overall structure, but, featuring a local spin-independent self-energy, it does not capture the dependence of the spectral weights on $k$ and on the spin. As we show in the following, this dependence is crucial to properly describe the transition from the Mott insulator to the Pauli metal.

A first understanding of these effects can be gained observing that the RSOC behaves as a $k$-dependent magnetic field and even a weak spin-orbit coupling is sufficient to induce a finite helical spin-polarization in the paramagnetic Mott insulator, where the carriers are localized and become extremely reactive to magnetic fields. This is apparent in Fig. 2(c-g), where we plot the spin-resolved spectral function, $A_{\pm}(\omega, k)$, at different energies for $k_y = 0$ and $k_x \in [-\pi, \pi]$. For these $k$-values the RSOC effective field points along the $y$ axis and the Green’s function can be easily diagonalized yielding $A_{\pm}(\omega, k) = A_0(\omega, k) \pm A_y(\omega, k)$ for the two helicities.

In Fig. 3 we show the evolution of the spectrum along two representative lines in the space of parameters which cross the insulator-to-metal transition. In the first row [Panels (a-e)] we show results for fixed $U = 6t$ and increasing values of the Rashba coupling $t_R$, while in the second row [Panels (f-j)] we fix a large value of the RSOC $t_R = 2t$ and we vary $U$ ranging from $U = 16t$ to $U = 2t$.

To trace the modifications and merging of the different bands we focus on the structure of the spectrum along $k_x$ and we plot the $\sigma_y$-component of the spectral function, $A_y(\omega, k)$.

In the absence of RSOC ($t_R = 0$) we recover a standard Mott insulator. Increasing $t_R$ the system at first remains in a Mott insulating phase but the two bands acquire a helical spin-polarization (Fig. 3(b)). A further increase of $t_R$ then induces a transition to a metallic state, (Fig. 3(c-d)) and, in the limit of large $t_R$ the effect of the interactions are strongly reduced and the spectrum strongly resemble the non-interacting one Figs. 3(e,i,j). Therefore, as $t_R$ goes from $0.5t$ to $2t$ the system undergoes a transition from a “helical” Mott insulator to a Rashba metal...
FIG. 4: Evolution of the spectral function $A_0(\omega, \mathbf{k})$ across the Mott transition for $t_R = 2t$ and $U \in [4t, 16t]$, Lorentzian broadening $\eta = 0.1t$ in the spectral function plots and $\eta = 0.25t$ in the DOS plots. The red arrows in panels (a,d) signal the appearance of rifts in the spectral function and the corresponding peaks in the DOS, these are the signatures of correlation in the Rashba metal, as we increase correlation (panels (b,e)) the rifts evolve into a pseudogap and eventually in the true Mott gap shown in panel (c,f).

Despite the interaction is unchanged to $U = 6t$.

On the other hand, at very large $U = 16t$ and large $t_R$, Fig. 3f, we find an insulating phase characterized by a flat spectrum with a very weak $k$ dependence, very different from that of the helical Mott insulator shown in Fig. 3b for a smaller $t_R$.

When $U$ is reduced, the non-interacting band-structure is recovered by merging the outer branches of the two bands, i.e. the positive helicity branch of the upper Hubbard band and the negative helicity branch of the lower Hubbard band. The inner branches progressively disappear across the transition. As shown in Fig. 3(d,h) the strong momentum dependence of the spectral weights implies that at the transition only some fragments of the inner branches remain and a pseudogap appears close to the $\Gamma$-point. The fragments of bands remaining around the high symmetry points are the hallmarks of strong correlation in the Pauli metallic phase. Their effects are visible not only in the spectral function but also in the Fermi surface where they lead to small pockets around the $X$-points.

To better understand what are the relevant energy scales governing the transition it is useful to consider the density of states (DOS) and its relation with the spectral function $A_0$ shown in Fig. 4. We start from the weakly correlated case shown in panel (a). In this limit the spectrum bears strong similarities with the non-interacting one. In particular, due to the presence of Rashba coupling, the Van Hove singularity at $\omega = 0$ characteristic of two-dimensional square lattices is split into two peaks, whose distance $E_0$, scales with $t_R$ as $E_0 = 4t(\sqrt{1 + t_R^2/t^2} - 1)$. At the same time two additional van-Hove singularities appear at the band edges with a distance proportional to the non-interacting bandwidth $W_0 = 8t\sqrt{1 + t_R^2/(2t^2)}$. The signatures of correlation, in this case, are the transfer of spectral weight at large $\omega$ associated with spin-wave excitations and the appearance of rifts at high-symmetry points yielding the two small peaks close to the Fermi level indicated with a red arrow in Fig. 4(a). As we increase interaction, the rifts evolve into pseudogaps (Fig. 4b) and they connect with the true Mott gap in the insulating phase as shown in Fig. 4(c). In this phase the four-peak structure characteristic of the non-interacting Rashba metal on the square lattice is reproduced in each of the two Hubbard bands. However, the changes in the bands dispersion induced by Hubbard interaction, clearly visible in Fig. 4(c), demonstrate a non-trivial renormalization of the different contributions to the kinetic energy.$^N$ We notice that cluster-Dynamical Mean-Field Theory studies of the two-dimensional Hubbard models have shown similar physics where the interactions give rise to different renormalizations of nearest-neighbor and further-range hoppings, leading to renormalizations of the Fermi surface$^{35}$ and appearance of the pseudogap and the superconducting gap$^{36}$.

We remark that, as we discussed above, the presence of RSOc affects the Mott transition in a much deeper way than a simple change in the bandwidth with respect to the $t_R = 0$ system. As discussed above, the RSOc yields a new screening mechanism of local interaction that changes the nature of the localization transition. To illustrate this point in Fig.4, we plot the Mott gap as a function of $t_R/t$ for a fixed value of $U = 8t$ and we compare it with the gap of an Hubbard model having the same bandwidth but no RSOc, i.e., with an effective spin-diagonal hopping amplitude, $t_{eff} = \sqrt{1 + t_R^2}/2$. It is clear that the gap of the Rashba system is remarkably smaller except for very small $t_R/t$ and it falls to zero at a relatively small value of the effective bandwidth, while the system without RSOc becomes a metal only at very large bandwidths. This clearly shows that the RSOc introduces a completely new screening mechanism which
 favors metallic phases. Figure 5 also demonstrate that in systems featuring a strong Rashba coupling and strong correlation small changes of $t_R/t$ may induce a transition from insulator to metal.\cite{34}

In this manuscript we have studied the interplay between a sizable Rashba spin-orbit coupling and Hubbard-like local interactions in a two-dimensional lattice model. We find that the RSOC strongly favors metallic phases, turning a Mott insulator into a Rashba metal through a transition which can not be described in terms of an effective standard Hubbard model with a renormalized kinetic term. The spectral properties reveal different mechanism in which the insulator transforms into a metal and underline a strong sensitivity of the spectral and transport properties on the value of the ratio between the RSOC and the standard hopping amplitude. Our results provide the community with simple and practical information about the strong effect of the spin-orbit coupling on Mott localization, which can be used as the cornerstone for the study of systems featuring simultaneously large RSOC and large Hubbard $U$ and as guidelines to tune and tailor the properties of these systems. The present work also triggers a number of interesting questions concerning the effects of inversion symmetry breaking and Rashba spin-orbit coupling on superconductivity in strongly correlated systems. In fact, while it is well-known that Rashba coupling may enhance electron-phonon superconductivity\cite{37,38} the effects of spin-orbit coupling on high-$T_c$ and unconventional superconductors are still to a large extent unknown.\cite{38}

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\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig5}
\caption{Red line: Mott gap as a function of the ratio $t_R/t$ shown on the lower horizontal scale for $U = 8t$. Blue line: Mott gap for $t_R = 0$, $U = 8t$ and an diagonal tunneling amplitude $t_{\text{eff}}$, shown on the upper horizontal scale.}
\end{figure}

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Supplemental Material to “Rashba-metal to Mott-insulator transition”

FIG. 6: Comparison between the interacting and non-interacting Fermi surfaces for $t_R = 2t$. Upper left and right panels show respectively the non-interacting Fermi surface and the Fermi surface for $U = 8t$. Lower left and right panels show the spin polarization of the states on the Fermi surfaces in the two cases.

FERMI SURFACE STRUCTURE

As we discussed in the main text, Rashba spin-orbit coupling favors the onset of a Pauli metallic phase in the two-dimensional Hubbard model. Depending on the strength of the Hubbard interaction, the Pauli metal may resemble strongly a simple uncorrelated Rashba metal or show the signatures of strong correlation. In Fig. 6 we show the Fermi surface of the Pauli metal at the transition where correlation effects are more prominent and we compare it with the Fermi surface of an uncorrelated 2D Rashba metal. Besides shrinking and symmetrizing the FS of the uncorrelated system, we notice that pockets appear at the points $X = \{\pm \pi, 0\}$ and $Y = \{0, \pm \pi\}$.

MOTT GAP AND KINETIC ENERGY

We now consider the dependence of the Mott gap and of the different contributions to the kinetic energy as a function of $U$. As one can see in Fig. 7 (left panel) in both cases the gap scales linearly with $U$ in the Mott phase, with a slope that is independent of $t_R$. The critical value of $U$ is instead strongly dependent on $t_R$. To further investigate the properties of the Pauli metallic and Mott insulating phases in Fig. 7 (right panel) we show the dependence of the Rashba and normal tunneling contribution to the kinetic energy as a function of $U$. The most significant effect is the discontinuity found at large $U$, related to a change of symmetry in the ground-state of the plaquette.

FIG. 7: Upper panel: Mott gap as a function of $U$ for $t_R = 0.5t$ and $t_R = 2t$. Lower panel: Rashba and standard (spin-diagonal) contribution to the kinetic energy and their sum as a function of $U$ for $t_R = 1.2t$.