Strong renormalization of the Fermi-surface topology close to the Mott transition

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The underlying Fermi surface is a key concept for strongly-interacting electron models and has been introduced to generalize the usual notion of the Fermi surface to generic (superconducting or insulating) systems. By using improved correlated wave functions that contain backflow and Jastrow terms, we examine the two-dimensional \( t-t' \) Hubbard model and find a non-trivial renormalization of the topology of the underlying Fermi surface close to the Mott insulator. Moreover, we observe a sharp crossover region, which arises from the metal-insulator transition, from a weakly interacting metal at small coupling to a resonating valence-bond superconductor at intermediate coupling. A violation of the Luttinger theorem is detected at low hole dopings.

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I. INTRODUCTION

The single-band Hubbard model with extended hopping on the square lattice has been widely investigated since the appearance of the high-temperature superconductors. Indeed, it is believed to represent the minimal model that is necessary to describe the electronic correlations in the Copper-Oxygen planes of Cuprate materials. A very rich variety of phases has been discussed in this context, including antiferromagnetism, superconductivity, charge-density waves, and non-Fermi-liquid metals. Studies with various numerical techniques, ranging from dynamical mean-field theory (DMFT) including its cluster extensions20 to quantum Monte Carlo techniques21–22 as well as analytic approaches23,24 have addressed hotly debated topics like the nature of the pseudo-gap phase or the superconducting correlations.

Landau15 and Luttinger16 have shown that the Fermi surface, which is the locus of gapless electronic excitations in \( k \)-space, represents a pivoting concept in the theory of Fermi liquids. The generalization of this notion for gapped systems (e.g., superconductors or Mott insulators) leads to the idea that there is an underlying Fermi surface that becomes gapped because of some symmetry breaking (leading to superconductivity) or electronic correlation (leading to a Mott insulator). In particular, the underlying Fermi surface can be defined by the locus of points where \( \text{Re}G(k,\omega = 0) \) changes sign \( (G(k,\omega) \) is the single-particle Green’s function), passing either to infinity (for usual Fermi liquids with well defined quasiparticles) or to zero.26 The question of determining the underlying Fermi surface is of central importance in strongly correlated systems, particularly in view of experiments with angle-resolved photoemission spectroscopy (ARPES).26 From the theoretical point of view, there are few attempts to study the topology of the Fermi surface in correlated systems; furthermore, they are limited to mean-field approaches27,28 including recent calculations with cluster DMFT29. Here, we make a substantial step forward and consider non-perturbative calculations directly in a two-dimensional system. We use variational wave functions containing backflow correlations, which have been shown to be very accurate in the Hubbard model29 and focus our attention on the topology of the underlying Fermi surface and the superconducting properties. We show that a strong renormalization of the underlying Fermi surface takes place close to half filling, when the Mott insulator is approached. In particular, the renormalization to perfect nesting occurring at the interaction-driven metal-insulator transition opens a new perspective on the crucial role of momentum dependence in describing the Mott transition.

At finite dopings we find a sharp crossover line, which emerges from the Mott-Hubbard transition point at half filling and separates a weakly-correlated metal and a strong-coupling superconducting state, in agreement with a recent observation of an unconventional metallic state at finite dopings.28 Our findings could be also related to a recently proposed first-order line separating two metallic phases, one with a pseudogap and one without.20 For the superconducting order parameter we obtain a sizable signal for moderately large on-site interactions, i.e., \( U/t \approx 7–10 \).

The paper is organized as follows: in section [II] we introduce the Hamiltonian and describe our variational wave function; in section [III] we present our numerical results and, finally, in section [IV] we draw the conclusions.

II. MODEL AND VARIATIONAL WAVE FUNCTION

We consider the Hubbard model with extended hopping on a two-dimensional square lattice,

\[
\mathcal{H} = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} - t' \sum_{\langle\langle ij \rangle\rangle} c^\dagger_{i'\sigma} c_{j'\sigma} + \text{h.c.} + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]  

(1)
FIG. 1: (Color online) Upper panel: variational hopping ratio \( \tilde{t}/\tilde{t} \) as a function of \( U/t \) for \( t'/t = -0.4 \) and \(-0.75\). Full (empty) symbols refer to the presence (absence) of backflow correlations in the variational wave function. Lower panel: variational hopping ratio \( \tilde{t}/\tilde{t} \) as a function of the doping \( \delta \) for \( U/t = 5 \) and 10 with \( t'/t = -0.4 \). Here, only results with backflow terms are shown. Data are shown for a \( L = 162 \) lattice; in the lower panel few points on a \( L = 242 \) lattice are added close to half filling.

where \( c^\dagger_{i\sigma} \) (\( c_{i\sigma} \)) denotes the electron creation (destruction) operator of one electron on site \( i \) with spin \( \sigma \). \( \langle ij \rangle \) and \( \langle(ij) \rangle \) indicate nearest and next-nearest neighbor sites respectively; \( n_{i\sigma} = c^\dagger_{i\sigma}c^{}_{i\sigma} \) is the electron density; \( t \) and \( t' \) are the nearest and next-nearest neighbor hopping amplitudes, and \( U \) is the on-site Coulomb repulsion. Calculations are performed on 45-degree tilted clusters with \( L = 2 \times 12^2 \) sites (\( l \) being an odd integer) and periodic boundary conditions. The number of electrons is \( N \), such that the hole doping is \( \delta = 1 - n \), with \( n = N/L \).

The question of determining the underlying Fermi surface has been addressed by using a renormalized mean-field approach in Refs. \[19\]-\[20\]. Here, we include electronic correlations in a non-perturbative way. In a first step, we construct uncorrelated wave functions given by the ground state \( |\Psi_{\text{BCS}}\rangle \) of a superconducting Bardeen-Cooper-Schrieffer (BCS) Hamiltonian\[27\]-\[28\]:

\[
\mathcal{H}_{\text{BCS}} = \sum_{k\sigma} \xi_k c^\dagger_{k\sigma} c^{}_{k\sigma} + \sum_{k} \Delta_k c^\dagger_{k+\mathbf{q}} c^{}_{-k-\mathbf{q}}^\dagger + \text{h.c.},
\]

where both the free-band dispersion \( \xi_k \) and the pairing amplitudes \( \Delta_k \) are variational functions. We use the parametrization

\[
\xi_k = -2\tilde{t}(\cos k_x + \cos k_y) - 4\tilde{t}'\cos k_x \cos k_y - \mu
\]
\[
\Delta_k = 2\Delta_{\text{BCS}}(\cos k_x - \cos k_y),
\]

where the effective hopping amplitude \( \tilde{t} \), the effective chemical potential \( \mu \), and the local pairing field \( \Delta_{\text{BCS}} \) are variational parameters to be optimized. The parameter \( \tilde{t} \) is kept fixed to set the energy scale. We also considered longer-range effective hopping parameters in Eq. (1), finding that all hoppings beyond the ones present in the Hamiltonian (1) are optimized to zero.

The correlated state \( |\Psi_{\text{BCS}}\rangle \), without backflow terms, is then given by

\[
|\Psi_{\text{BCS}}\rangle = J|\text{BCS}\rangle,
\]

where

\[
J = \exp(-1/2 \sum_{ij} v_{ij} n_i n_j)
\]

is a density-density Jastrow factor (including the on-site Gutzwiller term \( v_{ij} \)), with the \( v_{ij} \)’s being optimized for every independent distance \( |i - j| \). Notably, within this kind of wave function, it is possible to obtain a pure (i.e., non-magnetic) Mott insulator state, where the effective hopping amplitude \( \tilde{t} \) is zero, \( \mu = 0 \), and \( \Delta_{\text{BCS}} > 0 \) (\( \Delta_{\text{BCS}} = 0 \)).

A size-consistent and efficient way to further improve the correlated state \( |\Psi_{\text{BCS}}\rangle \) for large on-site interactions is based on backflow corrections. In this approach, each orbital that defines the unprojected state \( |\text{BCS}\rangle \) is taken to depend upon the many-body configuration, such to incorporate virtual hopping processes\[23\]-\[24\]. All results presented here are obtained by fully incorporating the backflow corrections and optimizing individually every variational parameter in \( \xi_k \) and \( \Delta_k \), in the Jastrow factor \( J \), as well as for the backflow corrections.

III. RESULTS

A. Fermi-surface renormalization

We start our analysis by discussing the evolution of the underlying Fermi surface topology as a function of hole doping \( \delta \) and interaction strength \( U/t \). Within the varia-
The location of the point $Q$ (in Fig. 1) is marked with an arrow.

For $t'/t = -0.4$ and $\delta = 0.025$, see Fig. 3. In summary, we present in Fig. 2 a complete description of the metallic phase. Then, at the metal-insulator transition, the variational hopping changes very rapidly by doping. Also in the metallic phase, the ratio $\tilde{t}/t$ is only slightly modified with respect to its bare value, and this result is found both with and without backflow correlations, demonstrating that even the simple wave function without backflow may capture a correct description of the metallic phase. Then, at the metal-insulator transition, the variational ratio of the hopping parameters is strongly renormalized in presence of backflow correlations, i.e., $\tilde{t}/t \to 0$, driving the underlying Fermi surface to be perfectly nested. This fact suggests that a full momentum resolution is a crucial ingredient to properly describe a metal-insulator transition. Remarkably, this renormalization does not occur if backflow correlations are not included. By further increasing the on-site Coulomb repulsion, the renormalized hopping ratio changes sign and then decreases again to zero at large $U/t$. This renormalization, which is again possible only in presence of backflow correlations, is in agreement with renormalized mean-field studies of the $t-J$ model where the Fermi surface renormalizes to perfect nesting for $\delta \to 0$, and with a slave-spin study of the Hubbard model in the large-interaction limit. Note that for $U/t > 25$ the numerical accuracy for the ratio $\tilde{t}/t$ is not enough to distinguish a finite from a vanishing value, see Fig. 1.

We would like to mention that a Fermi-surface renormalization close to the Mott transition has already been described in the one-dimensional Hubbard model. Also in that case, a perfectly nested Fermi surface, i.e., $k_F = \pm \pi/2$, is found. This consideration enforces the idea that the variational hopping ratio in two dimensions does not vanish accidentally at the Mott transition, but is renormalized in order to get perfect nesting of the underlying Fermi surface.

The variational hopping changes very rapidly by doping the Mott insulator and tends towards the bare value at high values of hole dopings, see the case $U/t = 10$ in Fig. 1. In summary, we present in Fig. 2 a complete density plot for the variational hopping $\tilde{t}/t$ as a function of doping $\delta$ and $U/t$, with bare $t'/t = -0.4$. While we have almost no renormalization when the half-filled case is metallic (i.e., for $U/t \lesssim 6$), we observe that a
The area enclosed by the renormalized Fermi surface, \( \tilde{\eta} \), and the number of electrons effectively present in the system, \( \bar{n} \), as a function of doping. Data refer to the case \( U/t = 10 \) and \( L = 242 \). Right panel: Same quantity as in the left panel as a function of \( U/t \) at half filling, for \( L = 242 \).

Strong renormalization close to half filling is present for \( U/t \gtrsim 6 \). Remarkably, the metal-insulator transition occurring at half filling comes with a sharp crossover line at finite doping that we can characterize through an abrupt change in the value of \( \tilde{\eta}/\tilde{\bar{n}} \). This crossover separates a weakly-correlated metal at low \( U/t \) and a strongly renormalized state at intermediate/strong values of \( U/t \). This result is in agreement with a recent ARPES study on YBa\(_2\)Cu\(_3\)O\(_{6+x}\), which found indications for an unconventional metallic state.\(^{25}\)

### B. Magnetic correlations

We provide here further evidence of the sharp crossover line by calculating the static spin-spin correlations, defined as

\[
S(q) = \frac{1}{L} \sum_{m,n} e^{i q (R_m - R_n)} \langle S_z^m S_z^n \rangle,
\]

where \( S_z^m \) is the \( z \)-component of the spin operator on site \( m \). The presence of (short-range) antiferromagnetic correlations is signaled by the appearance of a (non-diverging) peak in \( S(q) \), located at \( Q = (\pi, \pi) \). As shown in Fig. 3 for the doping \( \delta = 0.025 \), the correlated resonating-valence bond (RVB) state at \( U/t \gtrsim 6 \) is characterized by antiferromagnetic correlations that are strongly enhanced with respect to the metallic phase at \( U/t \lesssim 6 \). The two regimes are clearly separated by a jump in the value of \( S(Q) \); the short-range nature of the antiferromagnetic correlations is confirmed by a size scaling study.

### C. Momentum distribution function

In Fig. 3 we compare the results of the underlying Fermi surface with the ones for the momentum distribution \( n_k = \langle c_{k\alpha}^\dagger c_{k\alpha} \rangle \), for \( U/t = 10 \) and three different dopings. Interestingly, in the low-doping regime, the area enclosed by \( \xi_k = 0 \) is different from the one enclosed by the non-interacting system \( \xi_k^0 = 0 \), where \( \xi_k^0 = -2t (\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu_0 \), \( \mu_0 \) being the bare chemical potential. At half filling, the underlying Fermi surface is closed, but the system is insulating and consistently \( n_k \) shows a completely smooth behavior. This is due to the presence of a strong Jastrow factor \( v_q \sim 1/q^2 \) which is able to remove the singularities present in (BCS)\(^{26}\). As soon as a small doping is considered, the system becomes conducting and a finite jump in \( n_k \) appears along the nodal direction \( \Gamma \rightarrow M \), where the pairing amplitude \( \Delta_k \) vanishes. At small dopings, the variational hopping \( \tilde{t}/\tilde{t} \) undergoes an abrupt change (see Fig. 2 and, therefore, the Fermi surface becomes conducting and a full Fermi surface is recovered also in the momentum distribution, i.e., a finite jump is also detected along the \( M \rightarrow X \) direction. Additional results on the evolution of the underlying Fermi surface as a function of doping for \( U/t = 10 \) and \( U/t = 5 \) can be found in the Appendix A.

In the large doping case, the jump along the \( M \rightarrow X \) direction coincides with the position of the underlying Fermi surface. When the doping is small and there is no jump along the \( M \rightarrow X \) direction, one could extend the previous concept and associate the location of the maximal gradient of \( n_k \) with the position of the underlying Fermi surface. However, as shown in Fig. 4 this approach would lead to incorrect results, since the underlying Fermi surface is closer to the \( X \) point with respect to the location of the maximal gradient. Therefore, our results suggest that, when doping is small and electronic correlation is important, some caution should be taken in deriving the Luttinger surface from the location of the maximal gradient of \( n_k \) similarly to what has been discussed in Ref. 20 for the \( t-J \) model.
The renormalization of the underlying Fermi surface leads to a violation of the Luttinger sum rule. Let us denote by $\bar{n}$ the number of electrons that are enclosed by the renormalized Fermi surface $\xi_k = 0$. As shown in Fig. 4 close to half filling, the $\xi_k = 0$ contour is electron-like, containing less electrons than $n$, i.e., $\bar{n}/n < 1$, while for $0.05 \lesssim \delta \lesssim 0.2$, the contour is hole-like and $\bar{n}/n > 1$. For larger values of the doping, the Luttinger count holds. The summary for the Luttinger sum rule is reported in Fig. 9. Our results are slightly different from the ones found at the simple mean-field level\cite{43} especially close to the Mott insulator where we find that $\delta n \simeq -0.1$. In Fig. 5 we also present the violation of the Luttinger sum rule at half filling, as a function of $U/t$. In the insulating state ($U/t \gtrsim 6$) the underlying Fermi surface defined by $\xi_k = 0$ encloses less electrons than $n$. This result is compatible with the electron-like nature of the contour, due to the strong renormalization of the variational hopping parameters. On the contrary, in the metallic region we only observe a tiny violation, in particular close to the metal-insulator transition. This tiny violation can be related to the amount of correlation present in the low-$U$ metallic state and it is indeed significantly smaller than the degree of correlation that can be observed in the RVB state emerging from the Mott insulator upon doping, see Fig 9.

**D. Luttinger sum rule**

We discuss now the variational pairing amplitude $\Delta_{BCS}$, which measures the tendency to create resonating singlets, and the actual pair-pair correlations $\langle \Delta(r) \rangle = \langle S_r S_0 \rangle$, where $S_r = c_{r\uparrow} c_{r+\pi \downarrow} - c_{r\downarrow} c_{r+\pi \uparrow}$. At weak-coupling (when a conducting state is found at half filling), $\Delta_{BCS}$ remains relatively small and does not change much with doping, see Fig 9. For $U/t \gtrsim 6$ (when an insulating state is found at half filling), $\Delta_{BCS}$ has a sizable value and decreases monotonically as a function of the doping. This behavior of the pairing amplitude has been related to the pseudo-gap of the normal phase of Cuprate materials\cite{19}.

In Fig 7 we report the results for the superconducting order parameter $\phi^2 = \lim_{r \to \infty} \Delta(r)$, similarly to what has been done in previous calculations for the Hubbard and $t - J$ models\cite{40,45}. Our results are presented for $U/t = 7$ and 10, where superconductivity develops at finite doping. For smaller values of the on-site interactions, a much smaller signal is obtained. By increasing $U/t$, the optimal doping becomes larger and the magnitude of the order parameter decreases, suggesting that intermediate values of $U/t$ are optimal for maximal critical temperatures $T_c$, when assuming that $T_c$ scales with $\phi$.

**IV. CONCLUSIONS**

Our calculations represent a first attempt to trace the Fermi surface renormalization in a truly two-dimensional system where the electron-electron correlation is treated beyond simple mean-field approaches. A substantial deviation from the Luttinger sum rule is observed for large values of $U/t$, where the topology of the underlying Fermi surface changes from electron-like to hole-like by increasing the doping. It would be very interesting to verify these results on correlated materials, like Cuprate superconductors, where ARPES probes should be able to detect changes in the topology of the Fermi surface.

Furthermore, we show evidence of a sharp crossover region that originates from the metal-insulator transition and separates a weakly-correlated metal from a more correlated RVB superconductor at low dopings.

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**Appendix A: Underlying Fermi surface**

In Fig 8 we present a systematic plot of the underlying Fermi surface defined by the contour $\xi_k = 0$ and of the non-interacting Fermi surface, $\xi_k \bar{n} = 0$, as a function of
doping for the case $U/t = 10$. The underlying Fermi surface evolves from electron-like, when $\delta \lesssim 0.05$, to hole-like, for $\delta \gtrsim 0.05$. When $\delta \sim 0.2$ the underlying Fermi surface becomes very close to the non-interacting one, as expected when doping becomes large and electronic correlation consequently less important.

In Fig. 9 we present also a plot of the underlying Fermi surface as a function of doping for $U/t = 5$. In this regime, the half-filled case is metallic and the renormalization of the variational parameters is very weak. Consequently, the underlying Fermi surface does not show a remarkable evolution as a function of doping and almost coincides with the non-interacting contour.

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FIG. 8: (Color online) The underlying Fermi surface defined by $\xi_k = 0$ (solid blue lines) and the non-interacting Fermi surface $\xi_0^0 = 0$ (dashed black lines) as a function of doping. Data are presented at $U/t = 10$ for $L = 242$.

FIG. 9: (Color online) The underlying Fermi surface defined by $\xi_k = 0$ (solid blue lines) and the non-interacting Fermi surface $\xi_0^0 = 0$ (dashed black lines) as a function of doping. Data are presented at $U/t = 5$ for $L = 242$. 
