Dimensional-Crossover-Driven Mott Transition in the Frustrated Hubbard Model

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We study the Mott transition in a frustrated Hubbard model with next-nearest neighbor hopping at half-filling. The interplay between interaction, dimensionality and geometric frustration closes the one-dimensional Mott gap and gives rise to a metallic phase with Fermi surface pockets. We argue that they emerge as a consequence of remnant one-dimensional Umklapp scattering at the momenta with vanishing interchain hopping matrix elements. In this pseudogap phase, enhanced \(d\)-wave pairing correlations are driven by antiferromagnetic fluctuations. Within the adopted cluster dynamical mean-field theory on the \(8 \times 2\) cluster and down to our lowest temperatures the transition from one to two dimensions is continuous.

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The relative importance of spatial versus local fluctuations in the understanding of the Mott transition \([1]\) can be tuned with dimensionality. Starting from the high dimensional limit, experimental studies on \(\text{V}_2\text{O}_3\) indicate that exactly as a usual gas-liquid transition, the three dimensional bandwidth-controlled Mott transition belongs to the conventional Ising universality class: it is a first-order transition below the critical endpoint at \(T_c \approx 450\) K and affects solely the charge sector \([2]\). In contrast, Ising universality class has been ruled out in two-dimensional (2D) organic salts \(\kappa\)-(BEDT-TTF)\(_2\)X (BEDT-TTF: bis(ethylenedithio)tetrathiafulvalene, X: monovalent anion) with a much lower critical point \(T_c \simeq 40\) K \([3, 4]\). In this case geometric frustration, inherent to the triangular lattice, strengthens spin fluctuations which in turn affect the nature of the transition. The unconventional character of the quantum criticality in \(\kappa\)-(BEDT-TTF)\(_2\)X has been confirmed in recent numerical simulations \([5, 7]\). Moreover, enhanced spin fluctuations and spatial correlations in the copper oxide planes offer a natural framework which accounts for a depletion of low-energy states in the pseudogap regime of the high-\(T_c\) superconductors \([8, 10]\). As for the one-dimensional (1D) regime, it is dominated by spatial fluctuations \([11]\). The relevance of Umklapp scattering for the half-filled band leads to the absence of a bandwidth-controlled Mott transition. However, a Mott transition can be triggered as a function of dimensionality.

The aim of this Letter is to reexamine the dimensional-crossover-driven Mott transition in the quasi-1D Hubbard model at half-filling. The subject combines many fascinating issues such as the breakdown of spin-charge separation and the binding of spinons into magnons \([12]\). These phenomena follow from a delicate interplay between \(k\)-space and temporal fluctuations. To capture the relevant physics we employ a cluster extension of the dynamical mean-field theory (CDMFT) \([13]\). In the CDMFT, a cluster of \(N_c\) impurities is subject to a dynamical effective bath simulating the effect of all the other sites of the lattice \([14]\). The ability of the CDMFT to reproduce the density-driven Mott transition in the 1D Hubbard model has been demonstrated in Refs. \([15, 16]\). Previous CDMFT studies of the dimensional-crossover-driven Mott transition in weakly-coupled 1D chains yielded ordinary open Fermi surface (FS) in the Hubbard model \([17]\) and small FS pockets in the model of spinless fermions \([18]\).

We study the Hubbard model on a strongly anisotropic square lattice at half-filling,

\[
H = -\sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_{i\sigma},
\]

where the electron hopping \(t_{ij}\) is \(t (t_\perp)\) on the intrachain (interchain) bonds, \(\mu\) is the chemical potential and we set \(U/t = 3\). In addition, we allow for a finite diagonal next-nearest neighbor hopping \(t' = -t_\perp/4\) (see Fig. 1). It brings about frustration in the ground state and by reducing nesting properties of the FS precludes long-range magnetic order in the \(T = 0\) and weak-coupling regime \([19, 20]\). Hence, finite value of \(t'\) guarantees the Mott transition in the thermodynamic limit. We use the Hirsch-Fye Quantum Monte Carlo (QMC) algorithm as a cluster-impurity solver and extend previous studies \([17]\) to a low temperature regime. However, computational cost prevented us from decreasing the temperature below \(T = t/30\) on the \(8 \times 2\) cluster \([21]\). The CDMFT allows one to compute the single-particle spectral function \(A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G(\mathbf{k}, \omega)\). Here \(G(\mathbf{k}, \omega)\) is the lattice Green’s function represented in the original Brillouin zone. We estimate the latter by periodizing the cluster Green’s function and applying stochastic analytical continuation of the QMC data \([22]\).

Our main results are summarized in Figs. 1 and 2. The control parameter \(t_\perp\) interpolates between one and two dimensions and triggers the Mott transition at \(t_\perp/t \simeq 0.18\). To pin down the nature of the transition, continuous or first order, we plot in Fig. 1(a) \(\frac{\partial F}{\partial t_\perp} = \frac{1}{N} \sum_{\mathbf{k},\sigma} \frac{\partial \epsilon_{\mathbf{k}}}{\partial t_\perp} \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle\) with \(\epsilon_{\mathbf{k}} = -2(t \cos k_x + t_\perp \cos k_y) + \ldots\)
\( t_\perp \cos k_x \cos k_y \). Down to the considered temperatures, we do not detect a jump and thus conclude that the transition is continuous. \( \partial^2 F/\partial t^2 \) in Fig. 1(a) corresponds to an interchain charge susceptibility which is greatly enhanced in the vicinity of the critical coupling \( t_\perp /t = 0.18 \). The open warped Fermi lines which form at sufficiently large \( t_\perp /t > 0.24 \) (see Fig. 2) essentially follow from the topology of the tight-binding model. In the intermediate region, \( 0.18 \leq t_\perp /t \leq 0.24 \), we find a metallic phase where the FS is broken into electron and hole pockets.

On the one hand, starting from the 1D Mott insulating state, the occurrence of the pockets might be understood by taking the interchain hopping into account at the random-phase approximation (RPA) level \( [29] \). In this context the nodal points \( \mathbf{k} = (\pm \pi/2, \pm \pi/2) \) play a special role since \( \partial^2 U/\partial t^2 \) is zero there. On the other hand, starting from the large \( t_\perp \) limit, scattering off \( q_1 = (\pi, 0) \) and/or \( q_2 = (\pi, \pi) \) magnetic fluctuations could equally gap out the hot spots, \( \mathbf{k} = (\pm \pi/2, \pm \pi/2) \). To provide support for this scenario, we plot in Fig. 1(b) the cluster spin susceptibility \( \chi_s(q) = 1/N \sum_{\tau} e^{i q \cdot \xi} \langle S_{\tau}(\mathbf{q})S_{\tau}(0) \rangle \) for both momenta. As apparent, 1D fluctuations \( q_1 = (\pi, 0) \) remain robust up to \( t_\perp /t = 0.16 \) but are then gradually suppressed, giving way to dominant \( q_2 = (\pi, \pi) \) fluctuations, which peak at the Mott transition. Let us however note that in the static mean-field limit, antiferromagnetic order is not sufficient to reproduce the observed FS topology pointing towards the remnant 1D Umklapp scattering at the nodal momenta as the origin of the pockets.

Enhanced staggered magnetic fluctuations \( \propto \chi_s(\pi, \pi) \) give rise to pairing with a \( d \)-wave character \( \Delta^d_1(\tau) = \pm \sqrt{2} i c^\dagger_{i \uparrow}(\tau) c^\dagger_{i+\delta x \uparrow}(\tau) - c^\dagger_{i \downarrow}(\tau) c^\dagger_{i+\delta y \downarrow}(\tau) \) with the upper (lower) sign corresponding to \( \delta_x (\delta_y) \), respectively. The response of the system in the particle-particle channel is best seen in the pairing interaction vertex \( \chi_p^\nu \) \( [24] \). It is obtained from the full pairing susceptibility \( \chi_p = \frac{1}{N} \sum_{\tau} \langle \Delta^d_1(\tau)\Delta^d_2(\tau) \rangle \) by subtracting the uncorrelated contribution. As shown in Fig. 2(b), the calculated pairing vertex \( \chi_p^\nu \) is enhanced at the Mott transition.
which confirms the magnetic-pairing scenario.

The schematic evolution of the FS surface shown in Fig. 2(a) stems from the calculation of the single-particle Green’s function. In Fig. 2 we show the dimensionality-driven Mott transition as seen in the evolution of the single-particle spectral function $A(k, \omega)$. Most noteworthy features in the 1D limit shown in Fig. 2(a,b) are: (i) a well defined single-particle gap at $k = (\pi/2, 0)$ and equivalent points; (ii) signatures of spinon and holon branches especially in the vicinity of $k = (0, 0)$ [25], and (iii) backfolding of the energy bands around $k = (\pi/2, 0)$ and the equivalent points. Concerning (ii), already when $t_{\perp}/t = 0.15$ the intensity of the spinon excitation is noticeably reduced but nevertheless one can distinguish two peaks [26]. As shown in Fig. 3(c,d), they are superseded by a single peak with a broad shoulder at the Mott transition. Finally, a broad quasiparticle (QP) peak is resolved at $t_{\perp}/t = 0.2$ [26]. This remnant aspect of the 1D physics is captured in approaches starting from a fractionalized spectral function in the 1D limit and treating the interchain hopping at the RPA level [23, 27]. As for (iii), the pocket emerges when one of the backfolded bands intersects the Fermi energy. This defines a main and ghost side of the pocket which we can characterize with the magnitude of the QP residue $Z_k$. We extract this quantity by fitting the data to the Lorentzian form $A(k, \omega) \approx \frac{1}{\pi} \frac{Z_k \Gamma_k}{(\omega - E_{k} + \mu)^2 + \Gamma_k^2}$ and plot it in Fig. 3(b). At the exception of Mott transition at $t_{\perp}/t = 0.18$ where the pockets shrink and become very thin, strong anisotropy along the pockets is evident. We illustrate this in Fig. 4 by showing the low-frequency part of $A(k, \omega)$ across the pockets at $t_{\perp}/t = 0.2$. The two features — one with a large and the second one with a small QP weight crossing the Fermi level are part of the electron [Fig. 4(a)] and hole [Fig. 4(b)] pocket. The broken FS is unrelated to a specific ladder geometry of the $8 \times 2$ cluster and it is also found on the square $4 \times 4$ cluster [28].

The reconstruction of the FS is governed by the topology of the real part of the zero-frequency Green’s function $A(k, \omega)$ [29, 31]. In the Fermi liquid theory, $A(k, \omega)$ is positive (negative) inside (outside) the FS, respectively, and changes sign by going through a pole. This contrasts with the Mott insulator in which $A(k, \omega)$ changes sign in momentum space passing through a zero as a result of a diverging lattice self-energy $\Sigma(k, i\omega_m)$. We extract the latter from the Dyson’s equation $G^{-1}(k, i\omega_m) = G_0^{-1}(k, i\omega_m) - \Sigma(k, i\omega_m)$, where $G_0(k, i\omega_m)$ is the bare Green’s function, in combination with the spectral representation of the lattice Green’s function $G(k, i\omega_m) = \int d\omega \frac{A(k, \omega)}{\omega^2 - \omega_m^2}$. The diverging behavior of $\Sigma(k, i\omega_m)$ at momentum $k = (\pi/2, 0)$ in the Mott phase is shown in Fig. 5(a). It is the coexistence of infinities and zeros which accounts for the anisotropy of the emergent pockets. We focus on the electron pocket and illustrate this in Fig. 5(b) for $t_{\perp}/t = 0.18$. On the one hand, in close vicinity of the C-point with a vanishing $\Sigma(k, i\omega_m \rightarrow 0)$, two adjacent poles of $G(k, \omega)$ result in a very thin electron pocket. On the other hand, diverging $\Sigma(k, i\omega_m \rightarrow 0)$ yields a zero of $G(k, \omega)$ at the A-point. The latter reduces the QP weight of the nearby ghost side. The interference of the neighboring pole and zero becomes stronger with growing $t_{\perp}$ and prevented us from resolving the full structure of $G(k, \omega)$ already at $t_{\perp}/t = 0.2$. Indeed, at our lowest temperature $T = t/30$ only a pole associated with the main side of the pocket and a broad minimum in $G(k, \omega)$ is observed in Fig. 5(b). However, as depicted in Fig. 5(a) the ghost side remains visible in the spectral function. In analogy with the density-driven Mott transition in the 2D Hubbard model [29, 30], we believe that the emergence of a large FS above $t_{\perp}/t = 0.24$ corresponds to a simultaneous annihilation of the adjacent zero and pole leaving

![Image](image-url)
The pole carrying a larger QP weight.

We turn now to the nodal direction of the Brillouin zone. Figure 6 reveals that $G(\mathbf{k}, 0)$ remains almost unchanged with respect to the 1D regime up to the $\mathbf{k}$-selective Mott transition at $t_{\perp}/t = 0.18$. This agrees with: (i) the behavior of $\Sigma(\mathbf{k}, i\omega_m \to 0)$ at $\mathbf{k} = (\pi/2, \pi/2)$ which we expect to diverge in the $T \to 0$ limit up to $t_{\perp}/t = 0.2$, and (ii) the gap seen in $A(\mathbf{k}, \omega)$. On further increasing $t_{\perp}$, $G(\mathbf{k}, 0)$ develops a pole-like feature. As a result, a broad QP peak emerges at $t_{\perp}/t = 0.25$. Its weight is much smaller than that at $\mathbf{k}_F$ along the $(0, 0) - (\pi, 0)$ direction included for comparison in Fig. 6. The substantial variation in the scattering rate is a precursory indication of the broken FS at smaller $t_{\perp}$.

Let us expand briefly on a relationship of our results with real materials such as quasi-1D organic (TM)$_2$X salts where TM stands for TMTTF (tetramethyltetrathi-

The coherence temperature below which QPs form marks the crossover scale and vanishes at the critical point. At energy scales below the coherence temperature and in the close vicinity of the transition point, the FS topology shows hole and electron pockets. We attribute their origin to the remnant 1D Umklapp scattering at the nodal momenta. Such a mechanism can also account for the pockets observed in the spinless model [18]. The evolution of the pockets with $t_{\perp}$ can be understood by tracking the zero and poles of the single-particle Green’s function.

At energy scales above the coherence temperature, remnant features of spin-charge separation are apparent in the single-particle spectral function. At the two-particle level, the metallic state is characterized by enhanced antiferromagnetic fluctuations in the very close vicinity of the critical point. These magnetic fluctuations act as a glue for pairing correlations with a $d$-wave character. On the insulating side, the crossover scale is set by the Mott gap. Below this energy scale we observe robust 1D Mott physics: aspects of spin-charge separation are visible both in the spectral function and $(\pi, 0)$ magnetic fluctuations which remain intact. Further work aimed at investigating the finite temperature consequences of this quantum critical point is presently under progress.

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SUPPLEMENTARY DATA TO THE ARTICLE: DIMENSIONAL-CROSSOVER-DRIVEN MOTT TRANSITION IN THE FRUSTRATED HUBBARD MODEL

Figure 7 shows the single-particle spectral function $A(k, \omega)$ on the $8 \times 2$ cluster for $t_\perp/t = 0.15$ and $t_\perp/t = 0.2$ and it complements Fig. 3 in our Letter.

Auxiliary CDMFT simulations performed on the $4 \times 4$ cluster indicate that the broken FS is unrelated to a specific ladder geometry of the $8 \times 2$ cluster (c.f. Fig. 8). Hence, FS pockets appear to be a generic low-energy feature accompanying the Mott transition in the quasi-1D limit.

FIG. 7. Dimensional-crossover-driven Mott transition as seen in the spectral function $A(k, \omega)$ within the CDMFT on the $8 \times 2$ cluster: (a) $t_\perp/t = 0.15$ and (b) $t_\perp/t = 0.2$. Parameters: $U/t = 3$, $t' = -t_\perp/4$ and $T = t/30$.

FIG. 8. (color online) Low-energy part of the spectral function $A(k, \omega)$ at $t_\perp/t = 0.2$ within the CDMFT on the $4 \times 4$ cluster. Vertical bars track the position of the peaks constituting: (a) electron and (b) hole FS pockets. Parameters: $U/t = 3$, $t' = -t_\perp/4$ and $T = t/30$.