

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 8×2 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 V_2O_3 indicate that exactly as in 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 $T_c \simeq 450$ K and affects solely the charge sector [2]. In contrast, Ising universality class has been ruled out in two-dimensional (2D) organic salts $\kappa - (\text{BEDT-TTF})_2X$ (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 $\kappa - (\text{BED-TTF})_2X$ 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 \mathbf{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,

$$H = - \sum_{ij,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}, \quad (1)$$

where the electron hopping t_{ij} is t (t_\perp) on the intrachain (interchain) bonds, μ 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

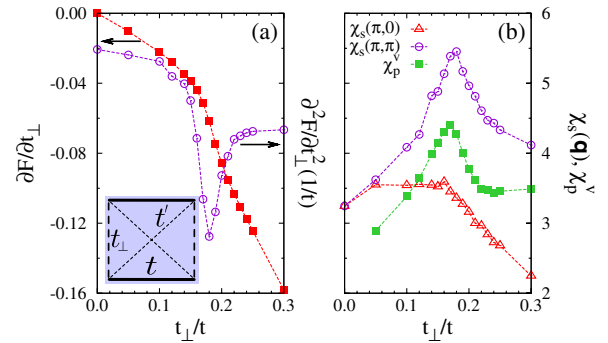


FIG. 1 (color online). (a) $\partial F / \partial t_\perp$ (squares) and susceptibility of interchain charge fluctuations $\partial^2 F / \partial t_\perp^2$ (scaled by a factor 0.1, circles); (b) spin susceptibility $\chi_s(\mathbf{q})$, and interaction vertex contribution to the d -wave pairing susceptibility χ_p^v (multiplied by 100) on the 8×2 cluster. Inset shows the lattice geometry of the Hamiltonian (1). Parameters: $U/t = 3$, $t' = -t_\perp/4$ and $T = t/30$.

the $T = 0$ and weak-coupling regime [19,20]. Hence, a finite value of t' guarantees the Mott transition in the thermodynamic limit. We use the Hirsch–Fye quantum Monte Carlo 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 8×2 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 quantum Monte Carlo 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 $t_{\perp}/t \approx 0.18$. To pin down the nature of the transition, continuous or first order, we plot in Fig. 1(a)

$$\frac{\partial F}{\partial t_{\perp}} = \frac{1}{N} \sum_{\mathbf{k}\sigma} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial t_{\perp}} \langle c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \rangle$$

with $\varepsilon_{\mathbf{k}} = -2(t \cos k_x + t_{\perp} \cos k_y) + t_{\perp} \cos k_x \cos k_y$. Down to the considered temperatures, we do not detect a jump and thus conclude that the transition is continuous. $\partial^2 F / \partial t_{\perp}^2$ in Fig. 1(a) corresponds to an interchain charge susceptibility that 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

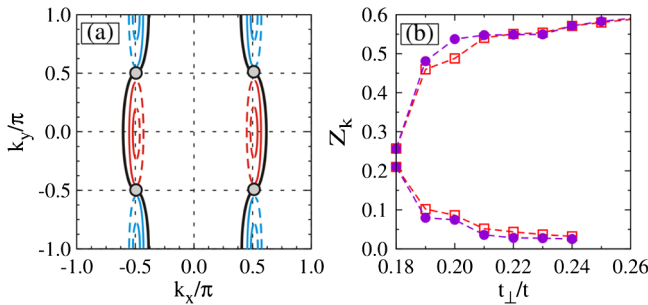


FIG. 2 (color online). (a) Schematic evolution of the FS. The emergent FS forms electron pockets around $\mathbf{k} = (\pm\pi/2, 0)$ and hole pockets around $\mathbf{k} = (\pm\pi/2, \pm\pi)$. The pockets have anisotropic distribution of the spectral weight between the main (solid lines) and ghost (dashed lines) vertical segments. The anisotropy and pockets' size grow until $t_{\perp}/t = 0.25$ when the ghost segments vanish and the main ones merge into the open FS of a quasi-1D metal (bold lines). The QP weight retains a strong \mathbf{k} dependence with a minimum at hot spots (dots). (b) QP weight $Z_{\mathbf{k}}$ on the main and ghost sides of the electron (squares) and hole (circles) pockets.

the interchain hopping into account at the random-phase approximation level [23]. In this context, the nodal points $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$ play a special role since $\partial \varepsilon_{\mathbf{k}} / \partial t_{\perp} = 0$ there. On the other hand, starting from the large t_{\perp} limit, scattering off $\mathbf{q}_1 = (\pi, 0)$ and/or $\mathbf{q}_2 = (\pi, \pi)$ 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

$$\chi_s(\mathbf{q}) = \frac{1}{N_c} \int_0^{\beta} d\tau \sum_{ij} e^{iq(i-j)} \langle S_i(\tau) S_j(0) \rangle$$

for both momenta. As apparent, 1D fluctuations $\mathbf{q}_1 = (\pi, 0)$ remain robust up to $t_{\perp}/t = 0.16$ but are then gradually suppressed, giving way to dominant $\mathbf{q}_2 = (\pi, \pi)$ 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 $\Delta_i^{\dagger}(\tau) = \pm \frac{1}{\sqrt{2}} [c_{i\uparrow}^{\dagger}(\tau) c_{i+\delta\downarrow}^{\dagger}(\tau) - c_{i\downarrow}^{\dagger}(\tau) c_{i+\delta\uparrow}^{\dagger}(\tau)]$ with the upper (lower) sign corresponding to $\delta = \mathbf{a}_x (\mathbf{a}_y)$, respectively. The response of the system in the particle–particle channel is best seen in the pairing interaction vertex χ_p^{ν} [24]. It is obtained from the full pairing susceptibility $\chi_p = \frac{1}{N_c} \int_0^{\beta} d\tau \sum_{ij} \langle \Delta_i^{\dagger}(\tau) \Delta_j(0) \rangle$ by subtracting the uncorrelated contribution. As shown in Fig. 1(b), the calculated pairing vertex χ_p^{ν} 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. 3, we show the dimensional-crossover-driven Mott transition as seen in the evolution of the single-particle spectral function $A(\mathbf{k}, \omega)$. Most noteworthy features in the 1D limit shown in Figs. 3(a) and 3(b) are, (i) a well-defined single-particle gap at $\mathbf{k} = (\pi/2, 0)$ and equivalent points, (ii) signatures of spinon and holon branches especially in the vicinity of $\mathbf{k} = (0, 0)$ [25], and (iii) backfolding of the energy bands around $\mathbf{k} = (\pi/2, 0)$ and the equivalent points. Concerning (ii), when $t_{\perp}/t = 0.15$ the intensity of the spinon excitation is already noticeably reduced but nevertheless one can distinguish two peaks, see Supplemental Material [26]. As shown in Figs. 3(c) and 3(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 random-phase approximation 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

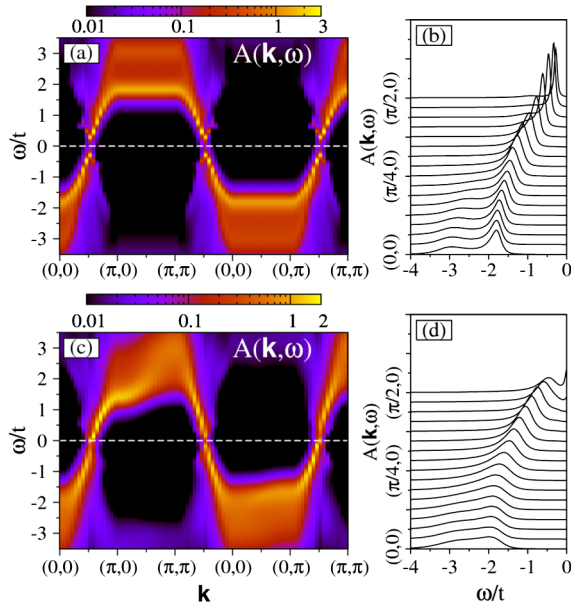


FIG. 3 (color online). Dimensional-crossover-driven Mott transition as seen in the single-particle spectral function $A(\mathbf{k}, \omega)$: (a, b) $t_{\perp}/t = 0$ and (c, d) $t_{\perp}/t = 0.18$. In panel (b), the spinon (holon) branch corresponds to the lower (higher) binding-energy peak, respectively.

magnitude of the QP residue Z_k . We extract this quantity by fitting the data to the Lorentzian form

$$A(\mathbf{k}, \omega) \simeq \frac{1}{\pi} \frac{Z_k \Gamma_k}{(\omega - \varepsilon_k + \mu)^2 + \Gamma_k^2}$$

and plot it in Fig. 2(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 $A(\mathbf{k}, \omega)$ 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)] pockets. The broken

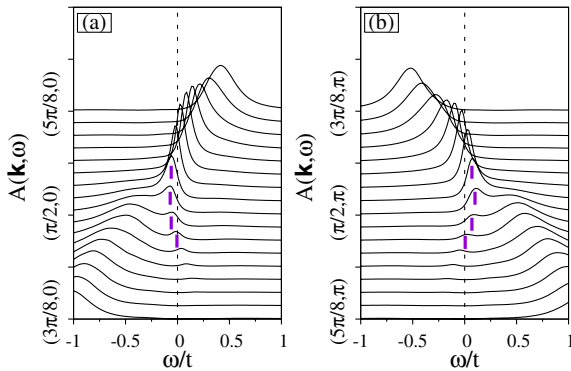


FIG. 4 (color online). Low-energy part of the spectral function $A(\mathbf{k}, \omega)$ at $t_{\perp}/t = 0.2$. Vertical bars track the position of the peaks constituting (a) electron and (b) hole FS pockets.

FS is unrelated to a specific ladder geometry of the 8×2 cluster, and it is also found on the square 4×4 cluster [26].

The reconstruction of the FS is governed by the topology of the real part of the zero-frequency Green's function $G(\mathbf{k}, 0)$ [28–30]. In the Fermi liquid theory, $G(\mathbf{k}, 0)$ is positive (negative) inside (outside) the FS, respectively, and changes sign by going through a pole. This contrasts with the Mott insulator in which $G(\mathbf{k}, 0)$ changes sign in momentum space passing through a zero as a result of a diverging lattice self-energy $\Sigma(\mathbf{k}, i\omega_m)$. We extract the latter from the Dyson's equation $G^{-1}(\mathbf{k}, i\omega_m) = G_0^{-1}(\mathbf{k}, i\omega_m) - \Sigma(\mathbf{k}, i\omega_m)$, where $G_0(\mathbf{k}, i\omega_m)$ is the bare Green's function, in combination with the spectral representation of the lattice Green's function $G(\mathbf{k}, i\omega_m) = \int d\omega [A(\mathbf{k}, \omega)/(i\omega_m - \omega)]$. The diverging behavior of $\Sigma(\mathbf{k}, i\omega_m)$ at momentum $\mathbf{k} = (\pi/2, 0)$ 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 $\Sigma(\mathbf{k}, i\omega_m \rightarrow 0)$, two adjacent poles of $G(\mathbf{k}, 0)$ result in a very thin electron pocket. On the other hand, diverging $\Sigma(\mathbf{k}, i\omega_m \rightarrow 0)$ yields a zero of $G(\mathbf{k}, 0)$ 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 $G(\mathbf{k}, 0)$, 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 $G(\mathbf{k}, 0)$ is observed in Fig. 5(b). However, as depicted in Fig. 4(a), the ghost side remains visible in the spectral function. In analogy with the density-driven Mott transition in the 2D Hubbard model [28,29], 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 the pole carrying a larger QP weight.

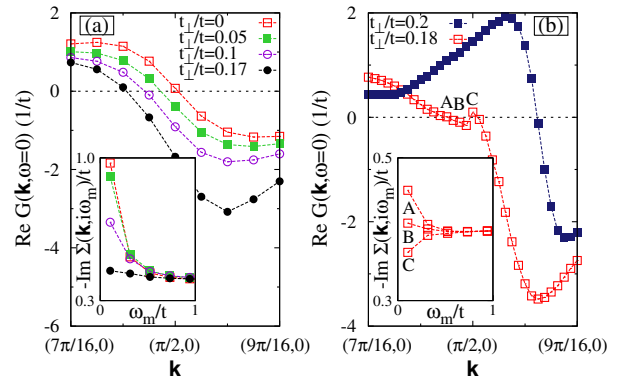


FIG. 5 (color online). Real part of the zero-frequency Green's function around momentum $\mathbf{k} = (\pi/2, 0)$ in the (a) insulating Mott phase and (b) metallic phase. Insets show the low-frequency imaginary part of the self-energy at $\mathbf{k} = (\pi/2, 0)$ in panel (a) and \mathbf{k} indicated by the capital letters in panel (b). $G(\mathbf{k}, 0)$ for $t_{\perp}/t = 0.2$ was rescaled by 0.5.

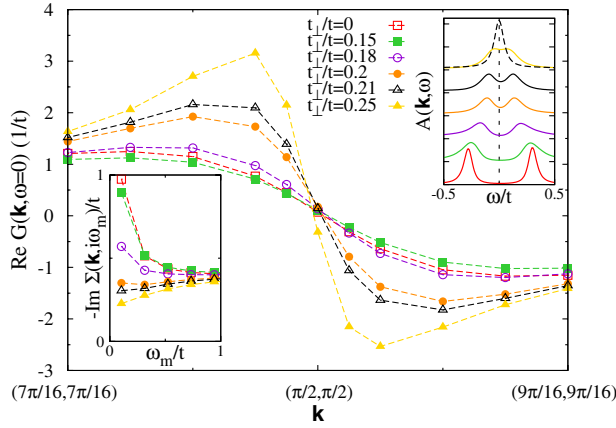


FIG. 6 (color online). Real part of the zero-frequency Green's function near the nodal $\mathbf{k} = (\pi/2, \pi/2)$ point. Insets show the low-frequency dependence of the imaginary part of the self-energy at $\mathbf{k} = (\pi/2, \pi/2)$ (left) and the corresponding spectral function from bottom ($t_{\perp} = 0$) to top ($t_{\perp}/t = 0.25$) (right). For comparison, dashed line in the right inset shows $A(\mathbf{k}, \omega)$ at \mathbf{k}_F along the $(0, 0)$ - $(\pi, 0)$ direction at $t_{\perp}/t = 0.25$.

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 $\Sigma(\mathbf{k}, i\omega_m \rightarrow 0)$ at $\mathbf{k} = (\pi/2, \pi/2)$, which we expect to diverge in the $T \rightarrow 0$ 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 polelike 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 $(\text{TM})_2\text{X}$ salts where TM stands for TMTTF (tetramethyltetrafulvalene) or its seleno TMTSF analogue [31]. Their unified phase diagram bears similarities to that of the high- T_c cuprates in the sense that as a function of pressure a superconducting phase emerges in the proximity of the insulating Mott phase. The inclusion of a finite t' in our studies mimics the unnesting role of pressure. As we show, crossing over from the 1D system to a higher-dimensional regime involves recombination of spinons and holons into the conventional QPs and releases the charge from the confinement to the 1D chains. The pressure-induced change in the optical spectroscopy data on $(\text{TMTTF})_2\text{X}$ is interpreted as an example of such a charge deconfinement [32,33]. A quantitative comparison would involve studies within a model Hamiltonian extended by electron-phonon coupling and long-range Coulomb interaction to account for a wide variety of phase transitions observed in the $(\text{TM})_2\text{X}$ families. Nevertheless, we find it encouraging that our CDMFT studies within the bare Hubbard model

of Eq. (1) support accumulating experimental evidence that superconductivity in the $(\text{TMTSF})_2\text{X}$ salts is mainly mediated by magnetic fluctuations [34]. Finally, the signatures of the closed FS contours that we find could be verified in quantum oscillation experiments.

In summary, our CDMFT simulations yield a continuous quantum phase transition between a 1D Mott insulating state and a 2D metallic state. On the metallic side, 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 in $(\pi, 0)$ 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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