Unusually thick metal-insulator domain walls around the Mott point

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Many Mott systems feature a first-order metal-insulator transition at finite temperatures, with an associated phase coexistence region displaying inhomogeneities and local phase separation. Here one typically finds “bubbles” or domains of the respective phases, which are separated by surprisingly thick, or fat, domain walls, as revealed both by imaging experiments and recent theoretical modeling. To gain insight into this unexpected behavior, we perform a systematic model study of the structure of such metal-insulator domain walls around the Mott point, within the Dynamical Mean-Field Theory framework. Our study reveals that a mechanism producing such “fat” domain walls can be traced to strong magnetic frustration, which is expected to be a robust feature of “spin-liquid” Mott systems.

I. INTRODUCTION

The Mott (interaction-driven) metal-insulator transition represents one of the most important phenomena in strongly correlated electron systems.1 It was first recognized in a number of transition-metal oxides,2,3 and has been brought to notoriety with the discovery of the cuprate high-$T_c$ superconductors,4,5 which raised much controversy surrounding its character and the underlying physical processes. One popular viewpoint, going back to early ideas of Slater, assumes that the key mechanism producing the Mott insulating state follows from magnetic order simply rearranging the band structure. An alternative perspective, pioneered by the seminal ideas of Mott and Anderson, argues that strong Coulomb repulsion may arrest the electronic motion even in the absence of magnetic order. Several theoretical scenarios6–12 have been proposed for the vicinity of the Mott point, but for many years the controversy remained unresolved.

More recent experiments have demonstrated13 that a sharp Mott transition is indeed possible even in the absence of any magnetic order. Physically, this possibility is realized in systems where sufficiently strong magnetic frustration14 can suppress magnetic order down to low enough temperatures, thus revealing the “pure” Mott point. Precisely such behavior is found in a class of organic “spin-liquid” materials,15 which have been recently recognized16 as the ideal realization of a single-band Hubbard model on a triangular lattice, allowing a remarkably detailed insight into the Mott transition region. While the intermediate-temperature metal-insulator crossover revealed17 some striking aspects of quantum criticality18 around the quantum Widom line,19 the transition was found to assume weakly first-order character at the lowest temperatures. Spectacular anomalies in dielectric response were observed20 within the associated phase coexistence region, revealing percolative phase separation.

Remarkably, most qualitative and even semi-quantitative aspects of the behavior observed around the Mott point were found to validate the predictions of Dynamical Mean-Field Theory (DMFT).21–23 This theoretical approach, which gained considerable popularity in recent years,24 focuses on the local effects of strong Coulomb repulsion, while disregarding certain nonlocal processes associated with inter-site magnetic correlations and/or fluctuating magnetic orders. It reconciled the earlier theories of Hubbard9,10 with the viewpoint of Brinkman and Rice25 leading to a consistent non-perturbative picture of the Mott point.

Figure 1: Spatial fluctuations of the local density of states (LDOS) found in a recent simulation of a moderately disordered two-dimensional Mott system, within the metal-insulator phase coexistence region.24 Note how the domain walls (green) covers a substantial area of the image, separating metallic (red) from the Mott-insulating domains (blue). Similar patterns have also been found in earlier imaging experiments on certain Mott oxides.26

While many aspects of crystalline Mott materials prove to be successfully described and interpreted from the perspective of DMFT, the situation is more complicated in the presence of disorder,27 which breaks translational invariance. These effects are most pronounced, but least understood, within the
metal-insulator phase coexistence region. Here even moderate disorder creates nucleation centers for the respective phases, leading to nano-scale phase separation. Some aspects of this behavior proved possible to be described from the perspective of a phenomenological percolation picture, including the effects of inhomogeneities caused by thermal fluctuations around the critical end-point, \[^{13}\] as well as the colossal dielectric response at lower temperatures.\[^{21}\]

A closer look at the microscopic structure of the corresponding patterns, however, revealed various puzzling features. Hints of remarkably complex behavior were provided by very recent large-scale numerical modeling\[^{23}\] of disordered Mott systems, as well as experimentally by nano-scale imaging of some Mott materials.\[^{6}\] A typical situation is illustrated in Fig. 1, where we reproduce a result of our recent theoretical study\[^{23}\] of this regime. Here we see clearly defined metallic domains separated from Mott-insulating regions by surprisingly thick domain walls, which in some cases cover a large fraction of the system volume (area). Remarkably, very similar fat domain walls were also observed in certain experiments,\[^{6}\] suggesting robust new physics. This finding immediately brings into question the conventional percolation picture, where the domain walls are assumed to play only a secondary role. This observation also brings forth several important physical questions, which are the primary motivation for this work: (1) What is the physical reason for having rather thick or fat domain walls, and under which conditions is this expected to hold? (2) What are the physical properties of such “domain wall matter”, and how should they affect the physical observables?

In this study we present a detailed theoretical investigation of the structure of such domain walls not only in the vicinity to the critical end-point,\[^{23}\] (where one generally expects them to be thick), but also across the entire phase-coexistence region. Our results establish that, under certain conditions, such domain walls can remain thick in the entire range of temperatures, and reveal the underlying mechanism, at least within the DMFT picture we adopt. We argue that strong magnetic frustration acts as a key physical ingredient affecting the properties of such domain walls, also suggesting ways to further control their properties in “materials by design”.\[^{15}\]

II. MODEL AND METHOD

To microscopically investigate metal-insulator domain walls in the vicinity of the Mott point, we focus on a single-band half-filled Hubbard model, as given by the Hamiltonian

\[ H = -t \sum_{\sigma} \left[ c_{i \sigma}^\dagger c_{(i+1) \sigma} + \text{h.c.} \right] + U \sum_i \left( n_{i \uparrow} - \frac{1}{2} \right) \left( n_{i \downarrow} - \frac{1}{2} \right), \]

where \( c_{i \sigma} \) (\( c_{i \sigma}^\dagger \)) is the creation (annihilation) operator of an electron with spin projection \( \sigma \) on site \( i \), \( t \) is the hopping amplitude between nearest neighbors, \( U \) is the on-site Coulomb repulsion, and \( n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \). We work in units such that \( \hbar = k_B = a = 1 \), where \( a \) is the lattice spacing. Energy will generally be given in the units of half-band width \( D \), which for our half-filled situation is also the Fermi energy.

In general terms, a domain wall in \( d \) dimensions is a \((d-1)\)-dimensional surface separating two thermodynamic phases. To examine its basic properties, we follow a standard procedure in assuming it to be flat, i.e. that its spatial variation across the wall is the only relevant one. To further simplify the calculation, we take advantage of the well-established fact that, within the DMFT formulation we employ, the detailed form of the electronic band structure does not qualitatively affect the results.\[^{19,20}\] This allows us follow the same strategy as in standard theories for domain walls, and reduce the problem to solving a one-dimensional model with appropriate boundary conditions on each end representing the respective thermodynamic phases.

![Figure 2: Schematic representation of the one-dimensional model we use to describe a domain wall. The central \( N \)-site sector, denoted as \( H_S \) in the Hamiltonian, contains the domain wall. It is attached to semi-infinite leads on both sides; a uniform, strongly correlated metal on the left and a uniform Mott insulator on the right. Both these reservoirs are described by the \( H_R \) term in the Hamiltonian. The \( N \)-site chain system is connected to the reservoirs through contact components, denoted as \( H_C \) in the Hamiltonian.](image-url)

To make our notation transparent, it is convenient to separate the Hamiltonian in three terms (see Fig. 2)

\[ H = H_S + H_R + H_C. \]

The first term \( H_S \) is a Hubbard Hamiltonian for the \( N \) central sites (“system”)

\[ H_S = -t \sum_{i=1}^{N-1} c_{i \sigma}^\dagger c_{(i+1) \sigma} + \text{h.c.} \]

\[ + U \sum_{i=1}^{N} \left( n_{i \uparrow} - \frac{1}{2} \right) \left( n_{i \downarrow} - \frac{1}{2} \right), \]

\( H_R \) refers to the semi-infinite chains to the left and to the right of the system (“reservoirs”)

\[ H_R = -t \left( \sum_{i=-\infty}^{0} c_{i \sigma}^\dagger c_{(i+1) \sigma} + \text{h.c.} \right) \]

\[ + U \left( \sum_{i=0}^{\infty} c_{i \sigma}^\dagger c_{(i+1) \sigma} + \text{h.c.} \right), \]

and \( H_C \) represent the coupling (“contacts”) of the central system to the reservoirs

\[ H_C = -t \sum_{\sigma} \left[ c_{0 \sigma}^\dagger c_{1 \sigma} + c_{N \sigma}^\dagger c_{(N+1) \sigma} + \text{h.c.} \right]. \]
In the following, we solve this model using Dynamical Mean-Field Theory (DMFT).\[12,21,29] The essential simplification of this approach is the assumption that the single-particle self-energy is a local but frequency-dependent quantity.[20] This self-energy is then calculated from the solution of an ensemble of auxiliary single-impurity problems supplemented with appropriate self-consistency conditions.\[20] Within DMFT, the Mott transition at half-filling exhibits a coexistence region where both the metal and the insulator represent locally stable thermodynamic phases. This coexistence region is delimited in the T vs. U phase diagram by two spinodal lines, $U_{c1}(T)$ (where the insulator becomes unstable) and $U_{c2}(T)$ (for the instability of the metal), as shown in Fig. 3. We further concentrate on behavior along the first order transition line $U_c(T)$ (green line in Fig. 3) where the free energies of the respective phases become equal.[15,16] To describe domain wall formation,\[18,41] we impose boundary conditions such that the sites to the left of the system are in the metallic phase, whereas sites to the right of it correspond to the Mott insulator. The intermediate region will then have to smoothly interpolate between metal and insulator, thus producing a domain wall between the two phases.

![Figure 3: DMFT phase diagram for the Mott transition at half-filling, obtained using IPT as the impurity solver. The phase coexistence region is bounded by the spinodal lines $U_{c1}(T)$ (blue line) and $U_{c2}(T)$ (red line) where the respective insulating and metallic solutions become unstable. The green line marks the first order transition line $U_c(T)$, where the free energies of the two phases coincide.](image)

Naturally, we will no longer able to assume a uniform, i.e., site-independent self-energy throughout the system. We will thus generalize the assumptions of DMFT to accommodate a non-uniform albeit still site-diagonal self-energy function

$$\Sigma(\omega) \rightarrow \Sigma_i(\omega).$$

This approach was first proposed in the context of a disordered system in Refs. [42] and [43] (for a review, see Ref. [44]. In the following, we explain the details of how the self-energy is computed for the present model. Like in the homogeneous DMFT, we focus on site $i$, whose dynamics, we assume, is that of a single correlated impurity site embedded in a bath of conduction electrons, whose action in imaginary time is

$$S_{\text{eff}}(i) = \sum_{\sigma} \int_0^\beta d\tau c_i^\dagger(\tau) \left( \partial_\tau - U/2 \right) c_i(\tau) + \sum_{\sigma} \int_0^\beta d\tau d\tau' \bar{c}_i^\dagger(\tau) \Delta_i(\tau - \tau') c_i(\tau') + U \int_0^\beta d\tau n_i^\dagger(\tau) n_i(\tau).$$

(7)

The hybridization function $\Delta_i(\tau - \tau')$ describes processes whereby an electron hops out of site $i$ at time $\tau'$, wanders through the rest of the lattice, and hops back onto $i$ at a later time $\tau$. We will specify how it is computed shortly. The local Green’s function of the impurity described by the action of Eq. (7) is

$$G_i(\tau) = -\left\langle T \left[ c_\sigma(\tau) c_i^\dagger(0) \right] \right\rangle_{\text{eff}}.$$

(8)

where the subscript $\text{eff}$ emphasizes that it should be calculated under the dynamics of Eq. (7). The self-energy $\Sigma_i(i\omega_n)$ is then obtained from the Fourier transform to Matsubara frequencies

$$G_i(i\omega_n) = \frac{1}{i\omega_n + U/2 - \Delta_i(i\omega_n) - \Sigma_i(i\omega_n)}.$$

(9)

The lattice single-particle Green’s function is given within this scheme by the resolvent (we use a hat to denote a matrix in the lattice site basis)

$$\hat{G}(i\omega_n) = \left[ i\omega_n - \hat{H}_0 - \hat{\Sigma}(i\omega_n) \right]^{-1}.$$

(10)

where $\hat{H}_0$ is the non-interacting Hamiltonian [Eq. (1)] with $U = 0$ and the matrix elements of the self-energy operator $\hat{\Sigma}(i\omega_n)$ in the site basis is

$$\left\langle i | \hat{\Sigma}(i\omega_n) | j \right\rangle = \Sigma_i(i\omega_n) \delta_{ij}.$$

(11)

The self-consistency loop is closed by requiring that the site-diagonal elements of the lattice Green’s function coincide with the local Green’s functions of Eq. (8)

$$\left\langle i | \hat{G}(i\omega_n) | i \right\rangle = \frac{1}{i\omega_n + U/2 - \Delta_i(i\omega_n) - \Sigma_i(i\omega_n)}.$$  

(12)

This last equation provides an expression for a self-consistent hybridization function for each site $\Delta_i(i\omega_n)$ in a completely homogeneous situation, the above scheme reduces to the standard DMFT.

The procedure described above requires the computation of the local Green’s function of Eq. (8) or, equivalently, the self-energy defined in Eq. (9) for the problem defined by the single-impurity action of Eq. (7). To this end, we utilized Iterated Perturbation Theory (IPT)\[30,43] as the required impurity...
solver. This procedure, while being computationally much more efficient than standard QMC methods, has previously been shown to properly capture both the insulating and the metallic solutions to the problem, as well as most other qualitative features of the full DMFT solution, which will suffice for our purposes.

If the system size $N$ is large enough to accommodate the full extension of the domain wall, the self-energy will be practically uniform in the region of the reservoirs. In carrying out our computations for different values of $U$ and $T$, we carefully verified that this condition is satisfied. For the parameter range explored in this work, $N = 50$ proved sufficient, except for the largest domain wall size we analyzed, for which a value of $N = 70$ was required.

Although the system studied is infinite, the computation of the local Green’s function and self-energy in the domain wall region is all that is required, as we now explain. It is easy to see that the non-interacting Hamiltonian $\hat{H}_0$ of the full infinite system has an obvious block structure given by

$$\hat{H}_0 = \begin{bmatrix} \hat{H}_S & \hat{H}_C \\ \hat{H}_C & \hat{H}_R \end{bmatrix}.$$  (13)

Likewise, the self-energy can also be separated into system $[\hat{\Sigma}_S (i\omega_n)]$ and reservoir $[\hat{\Sigma}_R (i\omega_n)]$ blocks

$$\hat{\Sigma} (i\omega_n) = \begin{bmatrix} \hat{\Sigma}_S (i\omega_n) & 0 \\ 0 & \hat{\Sigma}_R (i\omega_n) \end{bmatrix}.$$  (14)

The lattice Green’s function (10) satisfies the equation

$$\left[i\omega_n - \hat{H}_0 - \hat{\Sigma} (i\omega_n)\right] \hat{G} (i\omega_n) = \hat{1},$$  (15)

where $\hat{1}$ is the unit matrix. In block form, Eq. (15) reads

$$\begin{bmatrix} i\omega_n - \hat{H}_S - \hat{\Sigma}_S (i\omega_n) & \hat{H}_C \\ \hat{H}_C & i\omega_n - \hat{H}_R - \hat{\Sigma}_R (i\omega_n) \end{bmatrix} \begin{bmatrix} \hat{G}_S & \hat{G}_C \\ \hat{G}_C & \hat{G}_R \end{bmatrix} = \begin{bmatrix} \hat{1} & 0 \\ 0 & \hat{1} \end{bmatrix},$$  (16)

in terms of the (purely imaginary) self-energies on the left (metal) and right (insulator) $\Sigma_{L,R}$ blocks as

$$\hat{G}_{L(R)} (i\omega_n) = \frac{i}{2} \left\{ \Omega_{L,R} (i\omega_n) - \text{sgn}(\omega_n) \sqrt{\left[\Omega_{L,R} (i\omega_n)\right]^2 + 4r^2} \right\},$$  (24)

where $\Omega_{L,R} (i\omega_n) = \omega_n - \text{Im}\Sigma_{L,R} (i\omega_n)$.

In all our calculations we analytically continue the Matsubara Green’s functions and self-energies to the real axis using the Padé approximation.

### III. Results

Next, we present the detailed results we obtained, exploring the behavior of a domain wall within the coexistence region, in the entire range of temperatures $0 < T < T_c$, along the first-order transition line.

As we mentioned in Section II an accurate calculation needs to make sure that the system size $N$ is large enough so that our position-dependent solution converges to the proper asymptotic limit (“reservoirs”), where the spatial variation can be ignored. To illustrate this, in Fig.4 we display the domain wall profile, as described by the spatial variation of the local density of states (DOS) $\rho(0,x) = -(1/\pi) \text{Im} G(\omega = 0,x)$, evaluated at $T/D = 0.035$ and $U/D = 2.697$, and plotted as a function of the coordinate $x$ perpendicular to the domain wall. This quantity is small in the insulator (approaching zero as $T \to 0$), but remains finite in the metal, thus displaying strong spatial variation across the domain wall. As we can see in
The spatial variation of the local DOS $\rho(0,x)$ at the Fermi energy, across the domain separating a strongly correlated metal (left) and a Mott insulator (right), corresponding to $T/D = 0.0351$ and $U/D = 2.69773$. Results are shown for different system sizes $N$ used in our simulation, demonstrating negligible finite-size effects of our results.

Fig. 4, the spatial profile of the domain wall displays very little change with the size of the central region ($N$ sites), where we allow for spatial variation. This means that our system size $N$ is large enough to eliminate any finite-size effects from our calculation. Performing similar calculations for the different temperatures, we verified that $N = 70$ is sufficient for an accurate description at all the relevant temperatures ($0 < T < T_c$) within the coexistence region.

A. Anomalous dynamics of the domain walls

For each temperature we considered, we selected the precise value of $U(T)$ that falls on the first order transition line (see green line of Fig. 3). Results obtained for several temperatures are shown in Fig. 5 (a), showing the domain-wall profiles of the local DOS. We should mention that, within our simulation, the precise position of the domain wall we find for given $T$ and $U$, following the first-order transition line. Note a slightly non-monotonic dependence on temperature.
The corresponding behavior of the inelastic scattering rate
\[ \frac{1}{\tau}(0,x) = -2\text{Im} \Sigma(\omega = 0,x) \]
across the domain wall and different temperatures is shown in Fig. 7 (b). It is generally
expected to be small in a coherent metal (in a Fermi liquid
\[ 1/\tau \sim T^2 \]
for given U) and very large in a Mott insulator, as we
observe in the respective phases. This behavior reflects a
fundamentally different nature of transport in the two
competing phases, but even more interesting behavior is seen
within the domain wall itself. Here the scattering rate 1/\tau smoothly
interpolates between the two limits and thus retains very weak
\[ \propto T \]
dependence, reflecting significant electron-electron scattering
down to the lowest temperatures! This surprising result is
displayed even more precisely by plotting 1/\tau evaluated
at the domain wall center as a function of temperature, in
comparison to the behavior of the two phases, as shown in
Fig. 6 (b). Similar behavior is also seen in the frequency
dependence of the corresponding Green’s function and the self-
energy, shown as a function of the Matsubara frequency in
Fig. 7 for several sites across the domain wall at \( T = 0.035D \)
and \( U = 2.698D \). Here we observe a characteristic evolution
from metallic to insulating behavior, as one moves across the
domain wall, which is most pronounced at the lowest frequen-
cies. For the sites at the center of the domain wall, how-
ever, we observe characteristically weak frequency depend-
ence. This behavior is clearly distinct from either a metal or
an insulator, but is constrained by having to interpolate from
one to the other.

The domain wall center is, therefore, recognized as an inco-
erent conductor down to the lowest temperatures. Physically,
such non-Fermi liquid behavior makes it clear that the domain
wall represents a different state of matter from either a coher-
et (Fermi liquid) metal, or a Mott insulator. This surprising
result could be regarded as a curiosity with little physical con-
sequence in situations where the relative volume (area) frac-
tion “covered” by domain walls is negligibly small compared
to the bulk of the system. In the presence of sufficient dis-
order, however, both recent simulation \cite{23} and experiments \cite{26}
demonstrate a surprisingly abundant proliferation of such do-
main walls, suggesting a fundamentally new physical picture.
We may expect this to be especially significant whenever the
domain walls themselves are sufficiently fat (thick), so that a
sizeable fraction of the system’s volume (area) is affected by
such “resilient” inelastic electron-electron scattering, which
persists to low temperatures, in contrast to the behavior ex-
pected for conventional metals.

B. What controls the thickness of the domain walls?

To precisely quantify the domain wall thickness as a func-
tion of temperature, we fit its shape to the standard \[ \tanh(x/\xi) \]
form, generally found for domain walls separating two co-
existant phases \cite{36}. To be more precise, such symmetric do-
main walls of thickness given by an appropriate correlation
length \( \xi \) is what one expects near any finite-temperature crit-
ical end-point at \( T = T_c \), as we also find. At lower temper-
atures, however, our two phases are not related by any static
symmetry, hence the domain wall should not necessarily re-
tain its symmetric form, since the correlation length of the
respective phases may not be exactly the same. Indeed, even a
quick look at Fig. 6 (a) reveals that at lower temperatures, the
domain walls are much “thicker” on the metallic than on the
insulating side.

To quantify this behavior, we perform partial fits to the \[ \tanh(x/\xi) \]
form on each side of the domain wall center, which we
define as the corresponding inflection point in its profile.
Here \( \xi_x \), with \( a = \text{met or ins} \) defines the two different corre-
lation lengths, corresponding to the respective metallic or insu-
lating phase. The resulting \( T \)-dependence of \( \xi_{\text{met}} \) and \( \xi_{\text{ins}} \) is
shown in Fig. 8 (a), together with the total domain wall thick-
ness \( \xi = (\xi_{\text{met}} + \xi_{\text{ins}})/2 \). General arguments \cite{50}
predict this quantity to diverge at \( T \rightarrow T_c \), as we find.
Indeed, the critical point at \( T = T_c \) is known to belong to the Ising universality
class \cite{51}. According to an appropriate Landau theory \cite{20}
for this critical point, the domain wall width should be pro-
portional to the corresponding correlation length, diverging at
the critical point as \( \xi \sim \xi_{\text{corr}} \sim |T - T_c|^{1/2} \).
Remarkably, however, we find $\xi$ to display a divergence also at $T \to 0$, thus retaining a sizeable thickness even at intermediate temperatures. This behavior is seen even more precisely by plotting $\xi^{-2}$ as a function of $T$ in Fig. 8(b), displaying the expected square-root divergence not only at $T = T_c$ but also at $T = 0$. From the practical point of view, this curious result is important, because it suggests that domain walls should retain substantial thickness throughout the coexistence region, therefore introducing a potentially significant new feature of transport properties near the Mott point.

What could be the mechanism leading to this strange behavior? An important clue is provided by comparing the behavior of the corresponding correlation length describing the domain wall profile, as shown in Fig. 8(a). Here we observe that, while both $\xi_{\text{met}}$ and $\xi_{\text{ins}}$ diverge (and coincide) at $T \to T_c$, they behave very differently at $T \to 0$. Here $\xi_{\text{met}}$ diverges, but $\xi_{\text{ins}}$ saturates to a small value comparable to one lattice spacing. Physically, this result is easy to understand, keeping in mind the nature of the critical point at $U = U_c$, which we approach as $T \to 0$ along the first order line. This critical point signals the instability of the metallic phase, where the characteristic energy scale of the quasi-particles vanishes and the free energy minimum corresponding to the metallic phase becomes unstable, leading to the divergence of $\xi_{\text{met}}$. In contrast, the insulating solution here remains stable, as its own instability arises only at a much smaller $U = U_{c1} \ll U_{c2}$, and the corresponding $\xi_{\text{ins}}$ thus remains short, as we find.

The resulting behavior of the overall domain wall thickness $\xi = (\xi_{\text{met}} + \xi_{\text{ins}})/2$ is even more clearly seen by plotting $\xi^{-2}$ as a function of temperature, which is seen to linearly vanish both at $T = T_c$ and $T = 0$, as shown in Fig. 8(b). While domain walls are generally expected to become thick at finite-temperature critical end-points ($T = T_c$), the presence of such behavior also at low temperatures deserves further comment and a proper physical interpretation. Within our DMFT formulation, it reflects the emergence of an additional critical point at $T = 0$ and $U = U_{c2}$, corresponding to the divergence of the quasi-particle effective mass $m^* \sim (U_{c2} - U)^{-1}$, signaling a singular enhancement of the Sommerfeld specific-heat coefficient $\gamma = C/T \sim m^*$. This result, which is well-established within DMFT, reflects the approach to the Mott insulator characterized by large spin entropy at low temperatures. Physically, such neglect of significant inter-site spin correlations, as implied by the DMFT approximation, is expected to be justified in the limit of strong magnetic frustration, possibly in materials with triangular or Kagomé lattices.

IV. CONCLUSIONS

In this paper we performed a detailed study of the structure and the dynamics of domain walls expected within the phase coexistence region around the Mott point. Our results, obtained within the DMFT approximation, suggest that such domain walls should display unusual dynamics, which is unlike that of a metal or that of an insulator, locally retaining strong inelastic (electron-electron) scattering down to very low temperatures. This curious behavior could be significant in systems where weak disorder and low dimensionality conspire to produce a substantial concentration of domain walls within the metal-insulator phase coexistence region. This behavior should be especially significant in systems where the domain walls remain sufficiently thick or fat over an appreciable temperature range, such that the domain wall matter covers a substantial volume (area) of a given sample. Our predictions could be even more directly tested by STM (scanning tunneling spectroscopy) experiments, which are able to locally probe transport properties at the center of a given domain walls, in even simpler geometries.

Our analysis also revealed that the mechanism favoring such thick domain walls is directly related to the degree of magnetic frustration characterizing the incipient Mott insulating state. In spatially inhomogeneous systems (e.g. due to lattice defects of other forms of structural disorder), one can imagine local regions with varying degrees of local magnetic frustration. The physical picture we put forward indicates direct consequences for the structure of the corresponding domain walls, with their local thickness being a direct measure of the local magnetic frustration. The work we presented in this paper is only the first step in the investigation of situations where the interplay of phase coexistence, strong correlations, and magnetic frustration should lead to exotic forms of
dynamics of electrons, but more detailed investigations along these lines remain challenges for the future.

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APPENDIX: MOVING ALONG THE FIRST ORDER LINE

A close look at the results given in Fig. 5 reveals some details of the temperature dependence found, which deserve further clarification. It is clear that the DOS on the metallic side of the domain wall displays a noticeably non-monotonic T dependence, which is generally not expected for a metallic phase at fixed U. However, it should be noted that we have here the simultaneous variation of both T and U when we follow the first-order transition line (FOTL) while reducing the temperature. This complicates the analysis, producing the non-monotonic behavior, as we see even more clearly in Fig. 9. Note, in particular, that the metallic DOS does not approach the non-interacting value (horizontal dotted line), even at low temperatures, in contrast to what one finds by reducing T at fixed U (the so-called “pinning condition”, not shown).

To understand this behavior, we note that, at low temperatures, the metallic phase displays Fermi liquid behavior. In this case, all quantities become scaling functions of the reduced temperature \((T/T_{FL})\), where \(T_{FL} \sim Z/(U_c - U)\) is the Fermi liquid coherence scale and Z is the quasiparticle weight. Since, within DMFT, the FOTL also vanishes linearly with \((U_c - U)\), the reduced temperature \((T/T_{FL})\) should remain finite even as \(T \to 0\) along the FOTL line. This is the reason why the “pinning condition” is violated all along the FOTL. Indeed, within DMFT, the DOS is expected to approach its non-interacting value only at \(T \ll T_{FL}\), a condition that is not satisfied anywhere along the FOTL. The remaining T dependence we observe represents only sub-leading corrections, which are generally complicated and non-universal, consistent with the non-monotonic behavior we find.

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