Mott transition, Widom line, Frenkel line and pseudogap in the half-filled triangular lattice Hubbard model

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The Mott transition is observed experimentally in materials that are magnetically frustrated so that long-range order does not hide the Mott transition at finite temperature. Using the dynamical cluster approximation for the half-filled Hubbard model on the triangular lattice, we show that a) the Widom line that extends above the critical point of the first-order Mott transition exists in the thermodynamic limit; b) the presence of this line argues for the existence of the Mott transition in the thermodynamic limit; c) the loss of spectral weight in the metal to Mott insulator transition for strong interactions is momentum dependent, the hallmark of a pseudogap; d) the pseudogap to Mott insulator crossover line is a Frenkel line, analogous to the recently discovered crossover discussed in the statistical physics of the liquid-gas transition. Since the Mott transition and the liquid-gas transition are both in the Ising universality class, the Widom and Frenkel lines can be considered as very general emergent phenomena that arise in both ordinary liquids and electron liquids.

I. INTRODUCTION

The existence of a sharp Fermi surface (FS) and of quasiparticles at zero temperature in the presence of interactions is one of the remarkable emergent phenomena in strongly correlated electron systems. Correlation-induced insulating behavior is also an important emergent phenomenon. The transition from metal to Mott insulator (MI), called the Mott transition (MT), is considered a hallmark of strong electronic correlations in condensed matter physics. The simplest model that captures the MT is the Hubbard model \cite{1–5}. Recent reviews can be found in Refs \cite{6, 7}. Several numerical studies based on dynamical mean-field theory (DMFT) and its extensions \cite{8–13} have found that when interactions and kinetic energy become comparable, there is a MT, namely a first-order transition with hysteresis between a metallic and an insulating state \cite{8–19}. This was observed experimentally in materials \cite{20–25}.

Other emergent phenomena are associated with this first-order transition. Increasing the temperature $T$, the first order transition \cite{8–25} ends at a critical point \cite{16, 18, 19, 22, 26–29}, followed by a Widom line \cite{16, 19, 22, 26} in close analogy with phenomena in first-order liquid-gas phase transitions \cite{30, 31}. The Widom line acts as a high-temperature indicator of the underlying presence of a MT, sometimes hidden by long-range ordered states \cite{32, 33}.

One can wonder how far the liquid-gas analogy can be pushed. Recently, it has been found that the liquid-gas phase diagram contains another type of emergent crossover behavior in the supercritical state. This crossover occurs along what has been called the Frenkel line \cite{34}, a crossover line that does not begin at the critical point of the first order transition, contrary to the Widom line.

The Frenkel line is at the heart of debates over its definition and its origin \cite{34–38}. More specifically, it is argued that the Frenkel line should be either another Widom line, starting from the critical point, or a new line that would start below the critical point. In electron liquids, the Frenkel line has not been discussed before. It is thus important to accurately study all phenomena surrounding the MT.

The pseudogap (PG) is another important phenomenon associated with the Mott transition. Pseudogaps have been found in the $U$-$T$ phase diagram on the square lattice. Limiting ourselves to half-filling, for values of $U$ smaller than what is needed for a MT, the PG is a precursor of the long-range ordered antiferromagnetic (AFM) state \cite{39–44}. It appears when the AFM correlation length exceeds the thermal de Broglie wavelength, the so-called Vilk criterion \cite{39, 40}. If a PG also appears at half-filling when interactions are stronger than those needed for the MT, one should find out whether long AFM correlation lengths are also needed. In any case, in analogy with the finite-doping case, it would be useful to differentiate between the PG mechanisms for weak and strong interactions \cite{45, 46}.

In this paper, we study the normal-state phase diagram of the Hubbard model on the triangular lattice at half-filling. This model is appropriate for several experimental systems including organic conductors with $\kappa$-ET structure \cite{22, 24, 47–55}, some transition metal oxides \cite{56–58} or sulfides \cite{59}, cobaltates \cite{60} and artificial platforms like one-third monolayer of Sn atoms on a Si(111) surface \cite{61}, optical lattices \cite{62} and Moiré materials like twisted-bilayer graphene and transition-metal dichalco-
genides [63–68].

From a theoretical perspective, the triangular lattice offers the possibility to study the pristine finite-temperature normal-state phase diagram, including the Widom line, the Frenkel line, the PG and the MT, unencumbered by phase transitions to long-range ordered states. In particular, close to the value of $U$ where one finds the MT, a number of studies [15, 69–77], including a recent authoritative one [78], find that frustration is sufficiently strong to lead to a non-magnetic ground state, barring disagreement of variational calculations [79]. While superconductivity may arise [15, 29], it occurs at very low temperature. The absence of ordered states even at very low temperature also offers us the possibility to find out whether there is a PG at half-filling and, if there is one, to verify whether AFM is crucial for PG formation in the large $U$ limit.

We apply the dynamical cluster approximation (DCA) [11, 80] to the Hubbard model on a triangular lattice at half-filling. DCA is a cluster generalization of DMFT, detailed in Sec. II. In Sec. III, we unveil the $U$-$T$ phase diagram close to the MT, shown in Fig. 2. We prove at high temperature the existence of three phases: a correlated Fermi liquid (cFL), a MI and another one characterized by a momentum dependent loss of spectral weight, a strong indication of a PG phase. In Sec. IV, we present the first-order MT and, stemming from its critical point, a Widom line that extends at higher temperatures. We show how PG, cFL and MI phases compete around this critical point. We find in addition that the analog of a Frenkel line in classical statistical mechanics [34, 81] is a useful concept here to describe the crossover from the PG to a MI with a clearly visible gap. We also discuss the validity of our results with respect to the cluster choice, arguing that the results for the Widom line are valid in the thermodynamic limit. Since the Widom line emerges from the critical point that ends the first order MT, we argue that this also proves the existence of the MT in the thermodynamic limit, a result that has been recently questioned [78].

II. METHODOLOGY

A. The model.

One of the simplest and most studied model that incorporates both kinetic interactions on a lattice and strong local electronic correlations is the Hubbard model [6, 7, 82, 83], defined in second quantization as

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

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the operators that respectively create and annihilate an electron on site $i$ with spin $\sigma$, $\hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the corresponding number operator, $U$ is the energy cost of double occupancy, $\mu$ is the chemical potential and $t_{ij}$ is the kinetic energy of an electron hopping from site $j$ to $i$.

We allow hopping $t$ ($t'$) between $i$ and $j$ as nearest (next nearest) neighbors only, as depicted in Fig. 1 a), which presents the computational basis that we use for a triangular lattice. Every vertex represents a site and is connected to six neighbors by bonds that represent hopping. When $|t'|$ is equal to $|t|$, then the topology is exactly that of a triangular lattice shown in Fig. 1 b). On a square lattice, there would be another $t'$ hopping in the other diagonal direction.

Transformation between the computational basis vectors and the real-space basis vectors in Fig. 1 b) can be done with the combination of a linear transformation and a scale change, a special case of an affine transformation. The set of basis vectors $a_j$ and corresponding reciprocal lattice vectors $G_i$ in either the computational basis or the real-space basis satisfy $G_i \cdot a_j = 2\pi \delta_{ij}$. It is that property and the fact that the location of every site in the computational basis is obtained by exactly the same linear combination of basis vectors as in the real-space

![FIG. 1. (Color online.) a) Part of the triangular lattice in the computational basis. Note that only half of the bonds usually labeled $t'$ on the square lattice are considered, making this lattice topologically triangular. When $t' = |t|$, it is also physically triangular for all observables that do not require real-space representations. b) Part of the real-space triangular lattice. These two lattices can easily be mapped from one to the other by applying an affine transformation. c) Fermi surface of the triangular lattice in the computational basis for the non-interacting case at half-filling and for $t' = -t$. This figure shows how the Fermi surface is distributed among the patches of the $N_c = 6$ cluster. The white dots with an index in the middle of the patches are the allowed wave-vectors $K_i$ of the $N_c = 6$ cluster. d) Fermi surface and patches transformed to the real-space basis vectors in b). Note that patch 4 is at the center of a hole Fermi surface. The sign of $t$ is different in c) and d).](image-url)
basis that make the computational basis and the real-space basis generate identical dispersion relations. It is only at the end of the calculation, when there is a need to make predictions for scattering probes with actual wave vectors, that we need to transform back to the real-space basis, as in going from Fig. 1 c) to Fig. 1 d). Phase diagrams, that we focus on, are basis independent.

We work in units where $t$, $\hbar$, $k_B$ and lattice spacing are unity. Thus $U$, $t'$, $\mu$ and temperature $T$ are given in units of $t$.

**B. Solving the model.**

Although there is no known exact solution to the two-dimensional Hubbard model, DMFT captures the local quantum fluctuations generated by the large on-site Coulomb repulsion, which allows to solve it exactly in infinite dimensions [9, 84, 85]. In DMFT, the interacting atom of a lattice is mapped to an Anderson impurity model (AIM) embedded in an infinite bath of non-interacting electrons that describes the surrounding lattice. The dynamical hopping from the bath to the impurity and vice-versa is described by a hybridization function. The parameters of both the bath and the hybridization function are self-consistently determined by requiring that the self-energy of the impurity coincide identically with that of the infinite lattice.

However, since DMFT is exact only in infinite dimensions, it does not capture the spatial fluctuations that are quite important in the two-dimensional case we want to study. To correct this discrepancy, we use one of DMFT’s cluster generalizations, DCA [11, 80, 86].

In DCA, the Brillouin zone is divided into disconnected patches whose center is positioned at the coarse-grained wave vectors $K_i$. The wave vectors $K_c$ are the reciprocal lattice vectors of a small cluster with periodic boundary conditions. The wave vectors $k$ label every wave vector within a patch. We define $N$ as the number of wave vectors $k = K + \tilde{k}$ in the Brillouin zone and $N_c$ as the number of coarse-grained patches. With these definitions, the non-interacting dispersion relation in the cluster is defined using the average of the dispersion relation $\epsilon_k$ over each patch. The coarse-grained Green’s function in each patch is

$$G(K, i\omega_n) = \frac{N_c}{N} \sum_k G(K + \tilde{k}, i\omega_n).$$

The cluster self-energy $\Sigma_c(K, i\omega_n)$ for each patch is calculated as a functional of $G^{-1}_0(K, i\omega_n)$ defined by

$$G^{-1}_0(K, i\omega_n) \equiv \bar{G}^{-1}(K, i\omega_n) + \Sigma_c(K, i\omega_n)$$

that contains, here implicitly, the hybridization function. Self-consistency is achieved by modifying the hybridization function until the equality

$$\bar{G}(K, i\omega_n) = \frac{N_c}{N} \sum_k \frac{1}{i\omega_n - \epsilon_{K+k} - \Sigma_c(K, i\omega_n)}.$$
In order to systematically identify the cFL phase, we assume that the modulations of the one-particle propagator are not strong enough to convert the behavior of conduction electrons from itinerant to localized. Also, according to Luttinger’s theorem, one should expect a quasi-circular FS not to be very distorted by weak interactions. In other words, every patch that contains states at the Fermi level in the non-interacting case $U = 0$ should have their metallic-like behavior preserved, even in the presence of interactions. The DOS at the Fermi level in a given DCA patch $K_4$ is related to the Green’s function by

$$A(\omega = 0, K_4) = -2\text{Im} G(\omega \to 0, K_4).$$

Working with Matsubara frequencies $\omega_n$, the condition we selected to identify a cFL phase is $\text{Im}(G(i\omega_0, K_i)) < \text{Im}(G(i\omega_1, K_i))$ for every patch apart from $K_4$ since this patch does not have significant FS at $U = 0$ (see Fig. 1 c) and d)) and is thus not expected to be metallic at finite $U$. An example of this behavior in the cFL phase is again shown in the left panel of Fig. 2 c). As expected, this phase is found in the high-temperature and low-interaction strength regions of the phase diagram, where kinetic energy is dominant over potential energy. Lowering temperature, scattering decreases, resulting in an increase of the peak at Fermi level already present at high temperature (left panel of Fig. 2 b)). This can be deduced from Fig. 3 b) which shows the temperature-dependent spectral weight in the metallic state for $U = 8$. Recall that in a Fermi liquid, the lifetime becomes infinite at $\omega = 0$ and $T = 0$.

B. Mott insulator.

A key characteristic of a MI state is that it is completely gapped, leaving no spectral weight at $\omega = 0$. In Matsubara frequencies, we do not directly have access to this quantity. Instead, we extrapolate the three first Matsubara frequencies with a square fit to approximate the value of $-2\text{Im} (G(\omega = 0))$. We identify MI states in the phase diagram using the condition that this approximated value is smaller than 0.09. This somewhat arbitrary value comes from the limitations of the extrapolation. Using analytic continuation for the point marked with a downward triangle in Fig. 2 a), we also compute the DOS of the representative point of this phase shown in the right panel of Fig. 2 b), with the gap clearly seen.

Additionally, the loss of spectral weight characteristic of the MI should be visible for every wave vector and thus every DCA patch. This is observed for the representative point of the MI region of the phase diagram on the right panel of Fig. 2 c) and at the lowest temperature in Fig. 3 c). As expected during the MT, when we lower the temperature with $U > U_c$, we lose spectral weight on every patch until it becomes negligible. The shape of the MT and the Clausius-Clapeyron equation have implications for the understanding of the MI [19, 26]. This is discussed further in Sec. IV A 1.

C. Pseudogap.

We defined the cFL state in Sec. III A as having a quasi-particle peak at the Fermi level and metallic-like behavior for each DCA patch, while the MI phase in Sec. III B was defined as fully gapped at the Fermi level,
with each DCA patches having insulating character. This leaves us with an intermediary phase in Fig. 2 a) that we identify as PG.

The middle panel of Fig. 2 b) shows the DOS for a point in parameter space, marked by a diamond in Fig. 2 a), with PG features. There is no gap, but a dip indicating the absence of quasi-particles, a clear sign of a non-Fermi liquid behavior.

According to this criterion, this intermediary phase between the cFL and the MI could simply be classified as a bad metal as defined in Ref. [93]. In fact, two different phases are plausible: either a very small uniform gap or a PG. The only way to differentiate the two is to verify if the loss of spectral weight is either generalised on all the patches, for two different values of $U$. The phases are defined using the same criteria as in Fig. 2 a). Uncertainties are calculated using the error on the first Matsubara frequency and Ref. [94].

Additionally, one might have noticed that the patch loosing spectral weight the fastest is $K_0$, the only one with significant spectral weight that the AFM ($\pi,\pi$) Brillouin zone does not cross. This is relevant because for weak interaction strength, long-wavelength AFM fluctuations that are precursor to long-range AFM order lead to a PG at the crossing with the AFM Brillouin zone [97–99]. For sure, the many different orders possible at half-filling on the triangular lattice [71, 75, 100, 101] could lead to an analogous phenomenon, but it is unlikely. In any case, here we do not want to speculate further on the origin of the PG since this is not the main goal of this paper.

**IV. WIDOM LINE, FRENKEL LINE, PHASE TRANSITIONS AND CLUSTER CONVERGENCE**

In addition to the different phases identified in Fig. 2, the phase diagram contains a region bounded by lines labelled by $U_{c1}$ and $U_{c2}$. These spinodal lines correspond to values where observables such as the double occupancy, or equivalently the potential energy, show an hysteretic behavior between the cFL and MI phases, with a discontinuity characteristic of first-order transitions. Going up in temperature, $U_{c1}$ and $U_{c2}$ evolve and eventually connect at a critical point $(U_c, T_c)$ in parameter space, depicted
by a red star on the phase diagram. Although there is no longer a first-order transition above this temperature, the discontinuities that were present at the first-order transition along the spinodal lines now appear as an inflection point, forming a so-called Widom line [30, 102].

In Sec. IV A, we formally define the spinodal lines, the critical point and Widom line and discuss their appearance in the phase diagram of Sec. III obtained using the $N_c = 6$ cluster. We argue that the Widom line is a strong indicator of an underlying MT. In Sec. IV B, we provide a convergence study on the size and shape of the cluster, summarized in Fig. 5. It demonstrates unequivocally the existence of the Widom line in the thermodynamic limit, which in turn provides very strong evidence for the MT on the triangular lattice. This has been observed experimentally, for example, in layered organic conductors [22, 25, 51, 52].

A. Phase transitions and crossovers.

The MT is in the universality class of the liquid-gas phase transition [103, 104]. Both possess a Widom line and a first-order transition that ends at a critical point [16, 18, 19, 26–28]. In this section, we first discuss the first-order transition and then define and discuss the Widom and Frenkel lines.

We adopt the usual procedure to monitor double occupancy $D$ to find the first-order MT, Fig. 4 a) shows that at high temperature, double occupancy has an inflection point that turns, at low enough temperature, into a discontinuity with hysteresis, characteristic of a first-order transition. This situation is depicted on Fig. 4 b) for $T = 1/15$. The lower and upper boundaries in interaction strength of the resulting hysteresis are the spinodal lines labelled $U_{c1}$ and $U_{c2}$ in Fig. 2 a). As temperature decreases, $U_{c1}$ exhibits a sudden change in direction. There we find a small region of bistability between $U_{c1}$ and $U_{c3}$, namely two solutions with different double occupancy but similar DOS. This small region is further discussed in Appendix B. Calculating in this bistable region demands much more calculation time in order to stay in the insulating-like phases and this might be the reason why $U_{c2}$ appear to be at larger $U$ than its real minimum value.

Let us now compare the $U_{c2}$ line in Fig. 2 a) with that reported in previous works. Near the critical point where the first-order transition ends, this line behaves similarly to the one observed on square lattices [16, 19] where it was argued that this behavior reflects the fact that the entropy is smaller in the MI and PG phases compared to the cFL.

Following Ref. 26 to explain the slope of the first-order transition in our case, recall that the change in the free-energy at constant volume extracted from the partition function in the canonical ensemble is given by

\[
dF(T,N,U) = -s dT + \mu dN + D dU
\]

where $s$ is the entropy per number of sites. At half-filling ($n = 1$), along the line of thermodynamic phase transition $U_{pt}$ (found for the square lattice in Ref. 19) the free-energy in the cFL and the MI/PG states are equal, leading to $dT_{ins}/dU_{pt} = dF_{met}/dU_{pt}$. At half-filling, this implies the Clausius-Clapeyron equation

\[
\frac{dT}{dU} |_{U_{pt}} = \frac{D_{ins} - D_{met}}{s_{ins} - s_{met}}.
\]

Focusing now at the lowest temperatures, assuming that the slope of $U_{c2}$ follows that of $U_{pt}$ and extracting the inequality $\frac{dT_{c2}}{dU_{c2}} < 0$ from the $N_c = 6$ cluster in black in Fig. 5, we conclude that since the inequality $D_{ins} < D_{met}$ is satisfied, the thermodynamic entropy satisfies $s_{ins} > s_{met}$ as in single-site DMFT. Increasing temperature, the slope of the spinodal $U_{c2}$ becomes positive. Assuming again that this is the same trend as $U_{pt}$, either the numerator or the denominator of the Clausius-Clapeyron equation must change sign. Physically, we expect that the change in sign of the slope must come from a decrease in entropy at higher temperature, leading to the inequality $s_{ins} < s_{met}$. This is consistent with the result of Ref. [78] that increasing temperature increases 120 degrees spin correlations. It must manifest as a decrease of entropy of the paramagnetic insulating state.
There are plenty of different orders that could appear in a triangular lattice at low temperature [71, 105], a question we do not address here. But as mentioned in the introduction, for the range of $U$ where the first-order MT occurs, a number of studies [15, 69–78] find a non-magnetic ground state. Our calculations are in the paramagnetic state, so they are not accurate once true long-range order is established.

2. Widom line and critical point.

At high temperature above the critical point of the liquid-gas transition, thermodynamic quantities do not exhibit singularities. However, there are precursors of the first-order transition. Thermodynamic quantities, such as the specific heat for example, exhibit an extremum along a line that ends at the critical point. Different thermodynamic quantities yield different lines, but they all become asymptotically identical near the critical point, a consequence of the diverging correlation length [30, 31, 106]. Here we call the Widom line just the line associated with double occupancy, as we explain below.

Here we focus on the behavior of the double occupancy $D = \langle n_{\uparrow} n_{\downarrow} \rangle$, a first derivative of the free-energy with respect to interaction $U$, and on its derivative with respect to $U$, a second-order derivative of the free energy analogous to more usual thermodynamic quantities such as the compressibility [19, 102]. The corresponding Widom line is defined by

$$U_W(T, n) = \min_U \left( \frac{\partial D}{\partial U} \right)_{T, n}. \tag{8}$$

In other words, $U_W$ is the value of $U$ at fixed $T$ and occupation $n = 1$ where the change in double occupancy has a minimal value. Figure 4 a) show $D$ and its first two derivatives for an example case at $T = 1/8$ in the vicinity of the intersection with the Widom line. Because the change in curvature at the inflection point decreases with increasing temperature, the Widom line becomes difficult to determine. That line eventually becomes undetectable at high temperature so we did not investigate it for $T > 1/4$. With more precision and computing resources, the Widom line might be found at higher temperatures.

Using this method, we find the Widom line in the $T−U$ phase diagram at half-filling in the triangular lattice. It is identified in Fig. 2 a). We first note that it closely resembles what was found for various crossover lines on the square lattice using cluster DMFT (CDMFT) [16, 19, 102, 106]. Indeed, for $T > 0.2$ we find a negative slope, a rather constant slope for $0.14 < T < 0.20$ and a positive one for $0.11 < T < 0.14$. In Ref. 16, they argue that at temperatures above $T > 0.15$, the increased entropy of lightly correlated spins in the more localized phase favours that phase, leading to a negative slope. This is the sign of the slope found in single-site DMFT. Around $0.11 < T < 0.14$, the formation of singlets decreases the entropy of the more insulating phase compared with the metallic state, which explains the positive slope. Note that the MI/PG and the PG/cFL crossovers in the phase diagram of Fig. 2 a) all have positive slope. The more positive slope of the PG/cFL crossover line, compared with the MI/PG crossover line, suggests that the singlets in the PG region are more effective at decreasing the entropy compared with the cFL region than the singlets in the MI region are at decreasing the entropy compared with the PG region. In any case, this argument suggests that there are still many singlets in the PG region.

At the Widom line’s lowest point in temperature, we find the critical point, namely where $\partial D / \partial U \to -\infty$. At the critical point, the amount of correlations are largest and all extrema in thermodynamic quantities converge. The critical point’s coordinates obtained in this work are found to be a factor two larger than the one of Ref. 19 on the square lattice with nearest-neighbor hopping only. Increasing $|t'/t|$ on the anisotropic triangular lattice increases frustration and suppresses the Neel-AFM [71], concomitant with an increase in both $U_c$ [100] and $T_c$.

It is interesting to note, again in Fig. 2 a), that the critical point lies directly on the boundary between the PG and the cFL states. This PG/cFL crossover line is linked to the inflection point of a dynamical quantity, such as that of the total density of states, whose concavity at the Fermi level changes from a maximum to a minimum along a line [106] in the $U−T$ plane.

3. Frenkel line.

On the other hand, and perhaps surprisingly, the transition between the MI and the PG states does not pass through the critical point. There is however an analogous line in the liquid-gas transition called the Frenkel line [81], which usually starts from the first-order transition, below the critical point. Its main definition in the liquid-gas transition is that it separates regions where the liquid completely loses shear resistance at any frequency, becoming gas-like [34]. In particular, the velocity autocorrelation function loses all oscillatory behavior and decays monotonously.

In the context of the MT, what we call the Frenkel line separates a metallic-like state (PG) from an insulating-like one (MI). Taking the current-current correlation function used to compute the conductivity as the analogous of the velocity auto-correlation function, entering a gaped phase leads to a drastic change in behavior of the conductivity, a dynamical quantity. Note that this Frenkel line is very close to the line where cluster DMFT and continuous-time quantum Monte Carlo in the hybridization expansion found that the Mott gap becomes fully opened [106]. This line is almost independent of the type of cluster studied, which suggests that this is a very short-range effect. In addition, again in analogy with the Frenkel line in liquids, it extends to arbitrary values of temperature and of $U$ [106], contrary to the Widom line.
that in liquids becomes invisible at temperatures of order a few times the critical temperature.

**B. Mott transition and thermodynamic limit for the Widom line.**

The choice of the cluster labelled $N_c = 6$ shown in Fig. 5 a) for the results presented up to now is a compromise between the necessity to have a large cluster and the numerical resources required to perform the calculations. This cluster does not support three-sublattice order, is relatively small, although larger than many of the previously used clusters for the MT [16–18, 26, 106, 107], and following the definition of Ref. 108, is ferromagnetically imperfect when $t' = 0$. However, it is bipartite when $t' = 0$ (see Appendix A), a concept useful for strongly correlated systems [109]. When $|t'|$ is set equal to $|t|$, we recover the triangular lattice and the cluster becomes ferromagnetically perfect, as discussed in Appendix D. In this section, we compare the normal-state phase diagram obtained using this cluster with other cluster choices, summarized in Fig. 5.

For all the clusters in Fig. 5 a), the Widom line has been found and there is a clear trend that suggests that it survives in the thermodynamic limit. Although it is clearly seen for the largest $N_c = 16$ cluster at high temperature, we could not look for it below $T = 1/6$ in that cluster due to the long computation time and to the uncertainty coming from the sign problem (see Appendix A for further comments on the sign problem).

Since Widom lines were found only in small clusters before [19, 29, 32, 102], one could argue that they are an artefact. We claim that our results in Fig. 5 demonstrate that the Widom line exists in the thermodynamic limit [110].

The shape of the Widom line, which is consistent for all clusters except $N_c = 1$ (Fig. 5), is interesting. It starts from the critical point ($T \sim 0.1$) with a positive slope, following the trend of the phase boundary for the MT in clusters with an even number of sites. In such clusters, the formation of singlets in the insulator leads to smaller entropy in the insulator than in the metal [16]. The Clausius-Clapeyron equation Eq. (7) in turn imposes a positive slope. In all cases, at sufficiently high-temperature the slope becomes negative, as in single-site DMFT shown in Fig. 5 b), or more generally when there is an odd number of sites in the cluster [18, 106]. The odd number of sites leaves a net spin one-half in the insulator, which yields higher entropy in the insulator than in the metal thus yielding a negative Clausius-Clapeyron slope. Remarkably, the slopes of the Widom lines associated with double occupancy do become negative at the highest temperatures, suggesting that short-range superexchange interaction is not important anymore and that we have almost-free spin one-half degrees of freedom giving the same slope as in single-site DMFT. We do not understand why $U_W$ for single-site DMFT is so large. If the Widom line for $N_c = 1$ joins the other ones, it would be at very high temperature.

We did not seek to work on the detailed $U_{c1}$ and $U_{c2}$ for other clusters than $N_c = 6$ because previous papers already did [18]. Although patch and cluster definitions can impact final results [90, 91], our values of $U_{c1}$ and $U_{c2}$ are consistent with those of Ref. [18]. Neither did we feel that the $N_c = 6$ non-bipartite cluster would reveal important details for what we are looking for. Using the ladder dual fermion approximation, Ref. [111] finds that the system is insulating at $U = 10$. Additional results for the latter value of $U$ and a discussion of the disappearance of finite-size effects as a function of temperature may be found in Ref. [112].

FIG. 5. (Color online) Convergence with respect to the cluster size and shape. a) Five different divisions of the Brillouin zone. For each patch, the self-energy is calculated at the momentum $\mathbf{K}$ of its center, indicated by a black dot. We choose four lattice sizes: $N_c = 1, 4, 6$ and 16, with two different definitions for the 6 patches cluster: a non-bipartite one and a bipartite one, denoted by $N_c = 6^*$ and $N_c = 6$ respectively. What we mean by bipartite is discussed in Appendix A. The single site cluster corresponds to the DMFT case. b) Phase transitions of the different clusters of a). The dotted lines correspond to the Widom line $U_W$, the plain lines to the spinodals $U_{c1}$ and $U_{c2}$, and the dashed line to $U_{c3}$. The DMFT results are in a separate panel because the phase transitions are observed at much larger values of $U$. We only looked for $U_{c3}$ in the $N_c = 6$ cluster. The critical points, indicated by the red stars, are found in the same way as for Fig. 2. The coordinates of the critical points are $(U_{c1}, T_c)_{N_c=4} \sim (7.8, 0.10)$, $(U_{c1}, T_c)_{N_c=6} \sim (8.2, 0.11)$ and $(U_{c1}, T_c)_{N_c=6^*} \sim (8.5, 0.11)$. Error bars depend on the step in $U$ and on Monte-Carlo statistical noise.
V. DISCUSSION

The MT in Fig. 5 is found for a range of $U$ and $T$ consistent with that found previously in Ref. [18] for clusters of size $N_c = 1, 3, 4, 6$ and, for $N_c = 6^*$, with a different tiling of the Brillouin zone. On $2 \times 2$ plaquette square lattice clusters, CDMFT finds comparable values of $U$ for the MT [15, 95] while DCA with $N_c = 4$ clusters finds the slightly smaller value $U_c = 0.67$ at $T = 0.05$ [112, 113]. At the lowest temperature of $T = 0.1$ studied with CDMFT in Ref. [78], there is a sharp maximum in the kinetic energy for $N_c = 7$ around $U = 8 - 9$, but no jump indicative of a first-order MT. We argue that $T = 0.1$ is close to where we find the critical point. In addition, clusters with an odd number of sites are rather different from even numbered clusters, as the $N_c = 3$ results of Ref. [18] show. Odd numbers of electrons lead to an increased entropy coming from the $S = 1/2$ spin and the MT is tilted in the same direction as the $N_c = 1$ results, at odds with results with even numbered clusters that do not have this artificial degeneracy. The other methods used in Ref. [78] did not show a MT either, but the authors leave open the possibility that they cannot be conclusive on this point.

Results for lattices with slight anisotropy, $|t'|/t| = 0.8$, give similar ranges of values of $U$ and $T$ for the MT [27, 114]. The PG observed in weakly frustrated organics, $|t'|/t| \approx 1$, seems to originate from the long-wavelength spin fluctuation mechanism mentioned in the introduction [115]. This is different from triangular lattice organic compounds [116] that are more strongly correlated and where the PG physics may be more closely related to the one discussed here.

All clusters for which low temperature calculations could be done show a Widom line that ends at a critical point, followed by a MT. Hence, the Widom line is clearly a precursor to the MT. The inflection point in double occupancy is also seen in Ref. [78] at high temperature. The fact that the Widom line converges with system size suggests that the MT also survives in the thermodynamic limit.

For anisotropic triangular lattices, long-range order may hide the MT at the lowest temperatures as seen experimentally in organics [22, 50]. Nevertheless, a metal-insulator transition is seen above the long-range ordered states. Furthermore, in agreement with theoretical results on the triangular lattice for values of $U$ in the range where we see the MT [15, 69–78], experiments on organics show a MT separating a Fermi liquid and a spin liquid that is not hidden by long-range order [25, 51].

Finally, our results on the Frenkel line have connections to experiments. Indeed, measurements on quasi-two dimensional organic conductors suggest that the Frenkel line exists in strongly correlated materials. As can be seen on the MI side in Fig. 1 c) of Ref. 117 on organics, there is a range of temperatures below the critical point where the first-order transition is between two conductors. The material becomes truly insulating at a lower pressure (larger $U$) and higher temperature. The line that separates the conducting and insulating regimes has a positive slope in the $U - T$ plane and extends to large values of $U$ and $T$. We interpret this as the analog of the Frenkel line.

VI. CONCLUSION

We used DCA for the half-filled Hubbard model on the triangular lattice to study the Mott transition and how it influences the normal-state phase diagram in its vicinity. First, we demonstrated the existence of a Widom line in the thermodynamic limit by comparing results for different cluster sizes and boundary conditions. Second, we argue that the presence of the Widom line in the thermodynamic limit strongly suggests that the Mott transition also exists in that limit. Indeed, the Widom line always emerges at the end of the critical point of the first-order Mott transition. Third, we found that the Mott transition not only separates a correlated Fermi liquid from a Mott insulator, as found experimentally, it also separates the Fermi liquid from a region where a pseudogap appears. This pseudogap does not occur at AFM hot-spots, as is the case when spectral weight is lost due to long-wavelength fluctuations at small interaction strengths. Also, this pseudogap occurs on the large $U$ side of the Mott transition, instead of beginning on the small $U$ side, as is the case for the square lattice. Fourth and finally, pushing the analogy between the Mott transition and the liquid-gas transition, we found that the crossover line from the pseudogap to the Mott insulator follows the analog of a Frenkel line, which we argued has been observed experimentally.

This paper opens new areas of study. Having shown the existence of a pseudogap caused by strong interactions on the triangular lattice at half-filling, the next step should be to try to better characterize its underlying mechanisms and to look into the doped regime to find out if a similar pseudogap exists. Having shown that, on the triangular lattice, the Widom line, the Frenkel line, the Mott transition and the pseudogap are deeply interconnected emergent phenomena for strongly correlated electrons, experimental studies should now look for the concomitant presence of all four phenomena.

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Appendix A: Biparticity and sign problem.

In the case of the one-band Hubbard model with nearest-neighbor hopping, any infinite square lattice is bipartite which leads to particle-hole symmetry. Under that symmetry, one finds that \( n \rightarrow 2 - n \) and \( \mu \rightarrow U - \mu \) maps the results for the particle-doped lattices to those for the hole-doped ones. Thus by this symmetry, \( n = 1 \) when \( \mu = U/2 \). When the lattice is frustrated, this symmetry does not hold but a particle-hole transformation is still possible. In the computational basis Fig. 1 a), the infinite triangular lattice can be divided into 2 sublattices with \( t \) the inter-sublattice and \( t' \) (that we eventually set to \( -t \)) the intra-sublattice hopping terms. The particle-hole transformation then leads to the following statements about the clusters:

1. Changing \( -t' \rightarrow t' \) is equivalent to changing \( n \rightarrow 2 - n, \mu \rightarrow U - \mu \) and \( k \rightarrow K + (\pi, \pi) \);
2. Changing \( t \rightarrow -t \) is equivalent to changing \( k \rightarrow K + (\pi, \pi) \).

Within DCA, we verified thoroughly that this holds true for the \( N_c = 4, 6 \) and 16 clusters in Fig. 5, and not for the \( N_c = 6^* \) cluster. This is a manifestation of the fact that the \( N_c = 6^* \) cluster does not satisfy biparticity. Non-bipartite lattices have the attribute of enhancing frustration, thus inhibiting AFM order.

For \( t' = 0 \), we verified that our bipartite lattices are half-filled when the condition \( \mu/2 = U \) is satisfied while it is not for the non-bipartite lattice (for \( \beta = 20, U = 5.25 \) and \( \mu = 2.625 \), the filling is 0.995). In Fig. 6, we compare the filling as a function of the chemical potential for both clusters with six sites. The non-bipartite \( N_c = 6^* \) lattice does not display particle-hole symmetry. Although the high doping behavior is very similar on both sides, near half-filling it deviates from particle-hole symmetry. Using such non-bipartite cluster might be interesting to understand the general behavior, but isn’t as trust-worthy as bipartite ones.

Pushing further the analysis, we found some common behavior for all the clusters. Applying the particle-hole transformation by changing the sign of \( t' \), we noticed an important reduction in the average Monte Carlo sign, which was reduced by a factor two. In order to recover a better average sign, the hopping terms of a non-bipartite cluster needed to satisfy \( t \cdot t' = |t \cdot t'| \). In cluster DMFT, there are analogous choices of gauge that can increase the average sign [27].

Appendix B: Bistability.

In the coexistence region indicated by the hatched zone on Fig. 2 a), from the insulating phase, we have noticed a smaller zone where two solutions alternate. This is a typical behavior of the logistic map and it makes the insulating solution in the \( U_{c1} < U < U_{c3} \) range extremely unstable.

FIG. 6. (Color online) This figure displays three curves with \( t' = 0 \) where particle-hole symmetry should hold. The red curve is for the bipartite \( N_c = 6 \) lattice while the two others are for the \( N_c = 6^* \) non-bipartite lattice with and without the particle-hole transformation. The last two curves do not overlap, showing the lack of particle-hole symmetry of the \( N_c = 6^* \) cluster.

FIG. 7. (Color online) Left panel: Double occupancy as a function of iteration number for \( U = 7.97 \) and \( T = 1/15 \). The different colors give the parity of every iteration. The error bars are the Monte Carlo errors. Right panel: Density of state of the two alternating solutions of the left panel. This was made using the analytic continuation algorithm of Ref. 92. The color coding is identical for both figures.
To understand $U_{c3}$, we study a simulation performed in the $U_{c3} < U < U_{c3}$ region and illustrated on Fig. 7. On the left panel, we show the double occupancy as a function of the iteration number, where the even (odd) iteration numbers are plotted in cyan (red). We clearly notice the bistable phase is a feature that survives under DCA iterations and it strongly affects double occupancy. Even if we vary the weight of the last imaginary and real parts of the hybridization function, it does not change anything to the bistability gap. On the right panel, we plot the spectral weights obtained from analytic continuation of the Green’s function for the even and odd numbered iterations. Taking into account that analytic continuation is usually error prone, the DOS tells us that there ought to be little to no differences between the two cases. Hence, this may not be of importance for the pseudogap and does not cast doubts for our results outside this coexistence region.

Appendix C: Data compilation algorithm.

In order to compute the numerous average values and uncertainties presented in this work, we used the following algorithm. An observable $X$ calculated for $n$ iterations is given as an input. Its values and Monte Carlo errors at the $i^{th}$ iteration are labelled $x_i$ and $\sigma_{M,i}$. The result of each iteration is weighted by

$$w_i = 1/\sigma_{M,i}^2.$$  \hfill (C1)

With those, we calculate the weighted mean of the last $m$ iterations $\bar{x}_m$ using

$$\bar{x}_m = \frac{1}{w_{T,m}} \sum_{i=n-m}^{n} w_i \cdot x_i,$$  \hfill (C2)

where we defined $w_{T,m} = \sum_{i=n-m}^{n} w_i$ as the total weight from the $m^{th}$ iteration to the last one. We calculate the weighted uncorrelated standard deviation of the simulation as

$$\sigma_m = \sqrt{\sum_{i=n-m}^{n} w_i^2 \left( \frac{1}{w_{T,m}} \sum_{i=n-m}^{n} x_i^2 - \bar{x}_m^2 \right)}.$$  \hfill (C3)

Using the Confidence Interval Factor CIF(0.9999, $m$), we ensure that, in an uncorrelated simulation, we are 99.99% sure that $\bar{x}_m$ is inside the uncertainty. We define

$$\sigma_{CIF,m} = \sigma_m \cdot CIF(0.9999, m).$$ \hfill (C4)

From this, our algorithm aims to find the optimal $m$ ($m_{op}$) such that

$$m_{op} = \min \{ \sigma_{CIF,m} \}. \hfill (C5)$$

We selected $m \geq 15$, an arbitrarily limit made necessary by the correlations between iterations.

The output of our algorithm is the result $\bar{x}_{m_{op}}$ and we use $\sigma_{CIF,m_{op}}$ as the uncertainty.

Appendix D: Ferromagnetic imperfections.

Typically encountered in the context of ferromagnetism, the number of ferromagnetic imperfections $I_F$ relies on the concept of topological neighbors to predict the quality or goodness of a cluster with periodic boundary conditions \[108, 118\]. The importance of this concept in the context of strongly correlated electrons was emphasized in Ref. \[109\].

The Betts \[108, 118\] definition of perfect or imperfect finite-size cluster is as follows. First note that in an infinitely large square cluster, a site has four topological nearest neighbors, eight topological next-nearest neighbors, twelve third nearest neighbors and so on, with $4n$ $n^{th}$ nearest neighbors. For a given finite size cluster, all the $4n$ of the $n^{th}$ nearest neighbors of a given site may not be present on the cluster. As long as the $4(n-1)$ neighbors are all present, the cluster is perfect, unless further neighbors, such as those in the $(n+1)^{th}$ neighbor category, appear on the cluster.

The number of ferromagnetic imperfections $I_F$ of a cluster is defined as the number of displacements, or changes in the shape of the cluster, that are needed to make it perfect. Let us detail how $I_F$ can be counted on the square lattice ($I_{Fs}$) for several clusters shown in Fig. 8 a). They are the same as those defined in Fig. 5 a), with the addition of the cluster 16C from Ref. \[108\]. In the case of cluster 16C, starting from the site zero, we have four first neighbors, eight second neighbors and three third neighbors, thus $I_{Fs}(16C) = 0$. For the $N_c = 16$ cluster (which is the same as 16B in Ref. \[108\]), we have four first, six second, four third and one fourth neighbors, denoted (4,6,4,1). The number of ferromagnetic imperfections is given by the number of site displacements needed to build a perfect lattice. One can make a perfect lattice by doing the following displacements: (4,6,4,1) → (4,6,5) → (4,7,4) → (4,8,3). Since we did three displacements, $I_{Fs}(N_c = 16) = 3$. For each of our clusters, we find

$$I_{Fs}(N_c = 4) = 1,$$

$$I_{Fs}(N_c = 6^*) = 2,$$

$$I_{Fs}(N_c = 6) = 2,$$

$$I_{Fs}(N_c = 16) = 3.$$ \hfill (D1)

In Fig. 8 b), we illustrate how to extend the concept of ferromagnetic imperfections to triangular lattices, labelled $I_{Fs}$. In this configuration, a site in the infinite lattice will have $6n$ $n^{th}$ nearest neighbors. We find $I_{Fs}(16C) = 3$ while the clusters used in this work are all ferromagnetically perfect with

$$I_{Fs}(N_c = 4) = 0,$$

$$I_{Fs}(N_c = 6^*) = 0,$$

$$I_{Fs}(N_c = 6) = 0,$$

$$I_{Fs}(N_c = 16) = 0.$$ \hfill (D2)
FIG. 8. (Color online) Labelling of the intra-cluster topological neighbors of the site 0 for all clusters used in this work along with the cluster 16C from Ref. 108 for the a) square and b) triangular lattices. For each cluster, the super-lattice vectors are drawn in red.

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