Magnetic Correlations in the Two-dimensional Repulsive Fermi Hubbard Model

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The repulsive Fermi Hubbard model on the square lattice has a rich phase diagram near half-filling (corresponding to the particle density per lattice site \( n = 1 \)): for \( n = 1 \) the ground state is an antiferromagnetic insulator, at \( 0.6 < n < 0.8 \), it is a \( d_{xy} \) two-wave superfluid (at least for moderately strong interactions \( U \lesssim 4t \) in terms of the hopping \( t \)), and the region \( 1 - n \ll 1 \) is most likely subject to phase separation. Much of this physics is preempted at finite temperatures and to an extent driven by strong magnetic fluctuations, their quantitative characteristics and how they change with the doping level being much less understood. Experiments on ultra-cold atoms have recently gained access to this interesting fluctuation regime, which is now under extensive investigation. In this work we employ a self-consistent skeleton diagrammatic approach to quantify the characteristic temperature scale \( T_M(n) \) for the onset of magnetic fluctuations with a large correlation length and identify their nature. Our results suggest that the strongest fluctuations—and hence highest \( T_M \) and easiest experimental access to this regime—are observed at \( U/t \approx 4 - 6 \).

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The fermionic Hubbard model \([1,2]\), defined by the square lattice Hamiltonian

\[
H = -t \sum_{\langle i,j \rangle \sigma} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i \hat{n}_{i \uparrow} \hat{n}_{i \downarrow} - \mu \sum_i \hat{n}_{i \sigma} \quad (1)
\]

has for years played a crucial role in studies of correlated electrons in solids; it is regarded as one of the “standard models” of condensed matter physics to introduce and discuss Mott insulating phases, antiferromagnetic (AFM) correlations, novel mechanisms of superconducting pairing, non-Fermi-liquid behavior, etc. In Eq. (1) and in what follows, the nearest-neighbor hopping amplitude \( t \) is set to be the energy and temperature unit (distances are measured in units of the lattice constant); \( U \) is the on-site repulsive coupling constant; \( \mu \) is the chemical potential; \( c_{i \sigma}^\dagger \) and \( c_{i \sigma} \) create and annihlitate (respectively) a fermion of the spin component \( \sigma \in \{\uparrow, \downarrow\} \) on the site \( i \), and \( \hat{n}_{i \sigma} \) counts the number of fermions of a particular spin on a given lattice site.

On the one hand, Eq. (1) involves a number of crucial simplifications that make it qualitatively different from real materials, such as high-\( T_c \) superconductors. The most important ones include (i) strictly two dimensional (2D) as opposed to the strongly anisotropic 3D geometry, (ii) neglect of long-range Coulomb interactions, (iii) suppression of hopping matrix elements beyond the nearest-neighbor ones \((t' = 0)\), (iv) single-band approximation, and (v) absence of electron-phonon coupling. Correspondingly, the model \([1] \) cannot feature an ordered AFM phase at a non-zero temperature, but is allowed to have a first-order transition between phases with different electron densities, not to mention that \( t' = 0 \) leads to the Fermi surface nesting and particle-hole symme-

\[
\begin{align*}
&\text{Magnetic correlations} \\
&\xi \gg a \\
\end{align*}
\]

try at \( n = \langle n_{\uparrow i} + n_{\downarrow i} \rangle = 1 \). As a result, the schematic phase diagram of \([1] \) in the doping-temperature plane shown in Fig. 1 (see discussion below) is distinct from the “canonical” picture of high-\( T_c \)-type materials \([1] \). On the other hand, advances in ultra-cold atomic experiments have made it possible to accurately emulate the model \([1] \) on optical lattices \([5,13] \), bringing ultra-cold atom experiments into the region of the phase diagram (Fig. 1), where they can cooperate with the state-of-the-art numerical methods to reveal the underlying physics.

Figure 1. (color online). Schematic phase diagram of the repulsive Fermi-Hubbard model on the square lattice near half-filling, showing the Fermi liquid (FL), superfluid (SF), and phase separation (PS) regimes, as well as the antiferromagnetic ground state (AFM) at half-filling. Strong magnetic correlations with large correlation length \( \xi \gg a \) are observed below the dashed red line.
Numerical results can now be directly compared to experiments and vice versa dramatically increasing the importance of producing reliable data sets.

Recent years have seen a remarkable progress in unveiling the $T = 0$ phase diagram of the Hubbard model \cite{1}. Well-understood regions include the limit of vanishing densities $n \to 0$ \cite{14,20} and vanishing interaction strength \cite{21,24}. For densities $n \leq 0.7$ and coupling strength $U \leq 4$, the ground state is a BCS superfluid (with the $d_{x^2-y^2}$-wave symmetry at density $n > 0.6$) \cite{23}. At half-filling $n = 1$, the ground state is an AFM insulator for any $U$ \cite{25,30}. Being a qualitative property, AFM order can only disappear (with doping) by a quantum phase transition, with the simplest scenario being that of phase separation (PS). The first PS state was proposed to be a mixture of AFM and ferromagnetic (FM) orders in the region of small doping $\delta = 1 - n \ll 1$ and large $U$ \cite{31,33}; this conjecture has been later supported numerically for $U > 25$ \cite{34}. The instability of the model towards incommensurate AFM and domain wall formation was also reported in Refs. \cite{35,36}. Recently, PS for $U_n < U = 6$ \cite{31–33}; this conjecture has been later supported numerically for $U > 25$ \cite{34}. The instability of the model towards incommensurate AFM and domain wall formation was also reported in Refs. \cite{35,36}. Recently, PS for small values of $U$ was observed in Auxiliary-field Quantum Monte Carlo \cite{37,38} and variational \cite{39} studies.

Much less is known conclusively about the finite-temperature behavior. Given that the correlation length $\xi$ for AFM correlations at $n = 1$ diverges exponentially fast when $T \to 0$, there exists a relatively high temperature $T_M$ below which magnetic correlations extend over many lattice sites and electronic degrees of freedom are getting locked in collective modes. The characteristic temperature scale $T_M(n)$ is supposed to decrease with increasing the doping level. Since magnetic correlations and fluctuations are considered to be the prime reason for PS and BCS phenomena near $n = 1$, quantifying their behavior is paramount to understanding the finite-$T$ phase diagram of the Fermi Hubbard model in 2D.

In this Letter, we employ a skeleton diagrammatic approach to quantify the $T_M(n)$ scale, see Fig. 2 and shed light on the structure of dominant fluctuations. Experiments with ultra-cold $^6$Li fermions have now reached temperatures low enough to directly observe magnetic correlations in the model \cite{1,10,12}, with the lowest temperatures attained on the scale of $T \sim 0.25$ \cite{13}.

Method. The imaginary-time spin correlation function $\chi(\tau, i) = \langle S_z(\tau, i)S_z(0, 0) \rangle$ and its Fourier transform $\chi(\omega_m, \vec{q})$ at bosonic Matsubara frequencies $\omega_m = 2\pi T m$ ($m$ is an integer) was computed within the skeleton diagrammatic framework based on self-consistently renormalised (“dressed”) elements in four separate channels: particle-particle and particle-hole pair propagators, screened interaction, and single-particle propagator.

To define the framework, we first note that in the standard weak-coupling expansion in powers of $U$ (for introduction see, e.g., \cite{40}) every instance of the bare interaction vertex can be replaced by either of the three types of infinite sums shown in Fig. 3. These sums originate from three possible ways of connecting bare vertexes by non-interacting Green’s functions $G^{(0)}_{\sigma}$ to form a geometric series and are commonly referred to as particle-particle ($G^{(0)}_{pp}$), particle-hole ($G^{(0)}_{ph}$), and bubble (screened interaction $W^{(0)}_{\sigma\sigma'}$) ladders. Note that the functions $G^{(0)}_{pp}$, $G^{(0)}_{ph}$, and $W^{(0)}_{\sigma\sigma'}$, have the same structure as the single-particle propagators $G^{(0)}_{\sigma}$; i.e., thanks to the local nature of the Hubbard interaction $U$, they depend only on one lattice coordinate and time. Therefore, they are represented diagrammatically as lines, whereas the bare vertex is a point \cite{14}; the complete set of elements is shown schematically in Fig. 3 (left panel). An arbitrary diagram can now be constructed by taking any number of these elements and connecting their incoming and outgoing ends with
The resulting series contains significantly fewer terms because a large fraction of diagram topologies in the weak-coupling expansion are accounted for by the ladder sums.

\[
G_{\sigma} = \frac{G^{(0)}_{\sigma}}{1 - G^{(0)}_{\sigma} \Sigma_{\sigma}}, \quad W = \frac{U}{1 - U \Pi} - U , \quad (2)
\]

\[
G_{pp} = \frac{U}{1 - U \Sigma_{pp}} - U , \quad G_{ph} = \frac{U}{1 - U \Sigma_{ph}} - U , \quad (3)
\]

which are simple algebraic relations in the momentum/frequency representation. The diagrammatic calculation of self-energies built on the solutions of Eqs. (2), (3) for all the diagram lines is repeated iteratively until convergence. The spin-spin correlation function is then directly related to the polarization II by

\[
\chi(\omega_n, \vec{q}) = \text{Tr} \frac{\Pi(\omega_n, \vec{q})}{1 - \Pi(\omega_n, \vec{q}) U} S_z , \quad (4)
\]

with the trace taken over the spin index. This scheme can be abbreviated as \textit{GGGW} to emphasise the four renormalization channels.

To avoid double counting, diagrams for the self-energies must be constrained to the skeleton set in all the dressed channels: they must remain connected after cutting any two lines of the same kind; an example is shown in Fig. 4. In addition, one has to enforce two rules concerning dots: (1) no two dots can be connected directly by two Green’s functions, and (2) a dot cannot be connected by two Green’s functions to the same end of \(G_{pp}\) or \(G_{ph}\) or \(W\). This is necessary because, by construction, such diagrams are already accounted for in the corresponding ladder sums. Finally, there is one exception to the rule: to avoid triple counting of the same diagram contributing to the lowest-order \(\Sigma_{\sigma}\), one has to perform subtraction of the diagram based on two points, see Fig. 5.

\[
\Sigma_{\sigma}^{(1)} = \cdots + \cdots + \cdots - 2 \times \cdots + \cdots + \cdots = \cdots , \quad (5)
\]

\[
\Sigma_{pp}^{(1)} = \cdots + \cdots + \cdots - \cdots + \cdots + \cdots = \cdots , \quad (6)
\]

\[
\Sigma_{ph}^{(1)} = \cdots + \cdots + \cdots - \cdots + \cdots + \cdots = \cdots , \quad (7)
\]

\[
\Pi^{(1)}_{\sigma\sigma} = \delta_{\sigma\sigma} \quad (8)
\]

Figure 4. (color online). Diagrammatic elements based on ladders and screened interactions and an example of a particular diagram for the single-particle self-energy \(\Sigma\) based on them.

Figure 5. (color online). First-order skeleton graphs for all the self-energies evaluated in this work. The dressed lines in the diagrams are determined self-consistently by Eqs. (2), (3).  

All our results are based on the lowest-order GGGW scheme, in which the self-energies are given by the skeleton diagrams shown in Fig. 5 and the lines are computed self-consistently by Eqs. (2), (3). In principle, higher-order skeleton graphs can be summed by the standard diagrammatic Monte Carlo (DiagMC) scheme [25, 42–44] with obvious modifications required to handle a larger set of diagrammatic elements and self-energies. We have implemented the DiagMC scheme and used it to assess systematic errors of the lowest-order approximation.

Formally, the exact answer follows from summing the whole infinite series of all skeleton diagrams for the self-energies. However, it is known that in strongly correlated regimes close to half-filling \((U \gtrsim 4, T \lesssim 0.5, n \sim 1)\) skeleton sums for the Hubbard model cannot converge to the correct answer being attracted to an unphysical branch of the Luttinger-Ward functional [45]. On the other hand, at weaker interactions skeleton series quickly converge to the exact solution. Therefore, by continuity it is natural to expect that a low-order skeleton theory produces qualitatively and even quantitatively accurate results somewhat into the strongly correlated regime, provided the self-consistent dressing adequately captures fluctuations in relevant channels. We observe that it is indeed the case for the first-order GGGW approach employed here by benchmarking the results at \(n = 1\), which is notoriously the most difficult regime for skeleton schemes [45], against the numerically exact determinant diagrammatic Monte Carlo method [46, 47]. In particular, we observe that in the range or interaction strengths considered here, our approach produces accurate thermodynamic observables at the level of a few percent. The functional form of \(\Sigma_{\sigma}(\omega_n, \vec{q})\) and \(\chi(\omega_n, \vec{q})\) displays all the features and the deviation of the overall amplitude from the exact answer is at most 30%. For the purposes of the qualitative analysis carried out below this level of accuracy is sufficient. This makes the lowest-order GGGW scheme a practical
computationally-inexpensive tool that captures complex correlation effects in the regime of parameters accessible in current cold-atom experiments.

Results. The very notion of \( T_M \) as the crossover temperature between the high-temperature regime, in which the magnetic correlation length \( \xi \) is less than or comparable to the lattice constant \( a \), and the regime of strong long-range correlations with \( \xi \gg a \), implies that its definition is not unique. To characterise the onset of magnetic correlations we examine the momentum dependence of the static magnetic susceptibility \( \chi(\omega = 0, \vec{q}) \) and monitor development of a narrow peak structure. We define \( T_M \) at a given value of interaction \( U \) and density \( n \) as the highest temperature at which the amplitude of the peak in \( \chi(\omega = 0, \vec{q}) \) is an order of magnitude larger than its minimum value over the Brillouin zone, \( \chi_{\text{max}}/\chi_{\text{min}} = 10 \). Our results are summarized in Fig. 2.

As expected, the largest values of \( T_M \) (at fixed \( U \)) are observed at half-filling where the crossover temperature can be as high as \( T \sim 0.25 \) (or about 1000 K in units representative of the \( CuO_2 \) superconductors with hopping amplitude \( t \sim 0.3 \) eV [18]). As a function of interaction, \( T_M \) goes to zero at both large and small values of \( U \), and features a smooth maximum around \( U \sim 4 \). This appears to be the optimal spot for experimental studies of magnetism in the Hubbard model [1] where reaching low temperatures remains challenging. The magnetic crossover scale eventually goes to zero with doping but remains relatively high for intermediate values of \( U \) even at doping levels \( \delta \in (0.15, 0.25) \). We did not see evidence for PS at \( T_M \), meaning that the PS dome takes place within the magnetic region, see Fig. 1.

The character of spin correlations undergoes a dramatic transformation with doping. A mismatch between the largest momentum transfer at the Fermi surface and the reciprocal lattice vector results in the incommensurate spin-wave fluctuations that take the form of AFM domains with diagonal domain walls (or “diagonal carpet”, for brevity). In Fig. 5 we show a typical example of the emerging spin structure (for \( T = 0.05, U = 4 \) and \( n = 0.8085 \)). In the left panel, we see that the otherwise dominant peak around the commensurate vector \( (\pi, \pi) \) is split and features a minimum at \( (\pi, \pi) \) surrounded by two maxima at the incommensurate vectors. The real-space spin texture behind this split-peak signal is shown in the right panel with different colors corresponding to the sign of \( \chi(0, \vec{r}) \). It is plausible that in the PS region, see Fig. 1 the AFM order is intermixed with the diagonal carpet, and the mechanism for the \( d_{x^2−y^2} \)-wave pairing is based on coupling to these spin fluctuations.

Conclusions. We discussed the finite-temperature phase diagram of the repulsive Fermi Hubbard model on a square lattice and identified the overarching dome defining the onset of strong magnetic correlations that change their structure from commensurate antiferromagnetism to incommensurate diagonal texture as the doping level is increased. Given relatively high values of \( T_M \) that extend well into the doping region where optimal values for transition temperatures to the \( d_{x^2−y^2} \) superfluidity are expected to take place, magnetic correlations appear to be the key ingredient behind both the PS and superfluidity near half-filling.

Further development of the Diagrammatic Monte Carlo approach is required to obtain controllable results at temperatures below \( T_M \) where convergence of the diagrammatic expansion becomes problematic. Large magnetic correlation length and the possibility of phase separation should be treated with extreme care by any numerical method based on finite-cluster calculations because this physics imposes restrictions on the minimal acceptable cluster size and questions homogeneity of the solution. In particular, the superfluid states proposed in [15, 20] in the region of parameter space where one can expect phase separation [37–39] could result from the intrinsic bias of computational technique. To find high-\( T_c \) regions one has to avoid PS near half-filling by doping or modify the model to include non-zero values of the next-nearest-neighbor hopping \( t' > 0 \) [19].

Ultra-cold atom experiments are expected to have a major impact on revealing the finite-temperature phase diagram. Current experiments have already reached temperatures \( T \sim T_M \) [13], and are well positioned to explore the structure of strong magnetic correlations. Detection and characterization of the PS state requires reaching lower temperature scales. However, there is no a priori reason for the PS dome to take place at \( T \ll T_M \) given that known correlations saturate quickly below \( T_M \).

Quantifying magnetic correlations is also of significant interest in relation with copper oxides [51] as neutron scattering experiments have revealed the coexistence of commensurate and incommensurate magnetic structures at finite doping. For \( La_{2−p}Sr_pCu_4 \) an incommensurate
state with a magnetic structure wave vector was found at small dopings; for YBa$_2$Cu$_3$O$_{6+x}$ a wide doping window exists where commensurate AFM fluctuations are observed at low temperatures [52].

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