Charge Fluctuations in the Two-Dimensional Hubbard Model

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We investigate charge fluctuations in the two-dimensional Hubbard model as a function of doping, interaction strength, next-nearest hopping, and temperature within the eight-site dynamical cluster approximation. In the regime of intermediate interaction strengths, we find that d density wave fluctuations, which had previously been postulated using analytical arguments, are present and strong but cannot be interpreted as the cause for the pseudogap in the model, due to their evolution with doping and interaction strength. For all parameters away from half filling, the charge fluctuations investigated, including d density wave fluctuations, are weaker than d-wave superconducting fluctuations.

I. INTRODUCTION

The presence of large competing fluctuations of several kinds is one of the defining aspects of correlated electron systems. These fluctuations may then condense into phases that exhibit remarkable properties, including unusually high superconducting transition temperatures and interesting magnetism.

The cuprate superconductors are a paradigmatic example for such a competition. Antiferromagnetic fluctuations are strongest in the ‘undoped’ parent compounds but present over a large part of phase space. Superconducting fluctuations lead to a superconducting dome for dopings smaller than ~ 20%. Charge phenomena, such as the famous stripes at 1/8th doping or the features observed in scanning tunneling experiments, are present in several parts of phase space.

A minimal model that describes many of the salient features of these materials is the single-band Hubbard model. While unable to describe excitations involving high-lying orbitals, the model reproduces much of the observed low-energy phenomenology, including a pseudogap, superconductivity, and the response functions of Raman spectroscopy, optical conductivity, nuclear magnetic resonance, and neutron spectroscopy. It is therefore interesting to examine properties of the model in the context of cuprate physics. Due to the non-perturbative parameter regime relevant to the materials, reliable predictions have to resort to numerics, and a wide range of efficient numerical methods are able to describe the relevant parameter regime with consistent results.

Hubbard model calculations find spin-, charge-, and superconducting fluctuations. Spin fluctuations are well understood and mainly dominant near half filling. Calculations also find that strong short-wavelength spin fluctuations are primarily responsible for the formation of the pseudogap, i.e. the suppression of the density of states near the antinode but not near the node. Superconductivity is found unambiguously in the weak coupling regime, and strong indications from dynamical cluster calculations show that superconductivity does persist to larger couplings. In contrast, results from some newer methods find that in the absence of a next-nearest-neighbor hopping, it is charge (rather than superconducting) order that dominates the ground state. However, all orders are in very close competition. Currently, the precision to which the energetics of these phases is known is both substantially better than the critical temperature in experiment, when converted to the same units, and better than the uncertainty in the model parameters, indicating that phenomena beyond simple Hubbard model physics may well force the system to choose one order over the other.

At finite temperature, charge fluctuations, in contrast to antiferromagnetic and superconducting fluctuations, are less well investigated for the model without additional nearest-neighbor interactions, whereas the ‘extended’ model has been studied extensively in recent years. This is despite the fact that theoretical approaches have proposed unusual charge phenomena, such as the d density wave (DDW) order, as candidates responsible for pseudogap physics. It is therefore interesting to investigate the extent to which charge fluctuations are present in the model, and the extent to which they correspond to the proposed d density wave fluctuations, using numerical methods that generate these fluctuations dynamically from an underlying Hamiltonian. As we shall show below, the results are unexpected. First, we do find substantial d density wave fluctuations. However, while we find no area in parameter space where those fluctuations are dominant, they are comparable in magnitude to superconducting fluctuations (DSC). Also, while fluctuations are large in the general area of the pseudogap, the behavior with doping, interaction strength, and next-nearest neighbor hopping is not consistent with d density wave fluctuations as a mechanism for the suppression of the density of states.

The remainder of this paper is organized as follows. In section II we describe the method used in this paper. In section III we show the comparison between leading fluctuations in 2D Hubbard model. In section IV we show the temperature evolution of DDW and DSC. In section V we show the nearest hopping evolution of DDW. Section VI and VII discuss our results and present conclusions.
II. METHOD

We investigate the two-dimensional Hubbard model on a square lattice with on-site interaction $U$ and chemical potential $\mu$,

$$H = \sum_{\kappa \sigma} (\varepsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Here $i$ labels the lattice site, $k$ the momentum, $c^{(i)}$ annihilation (creation) operators, and $n$ the density, $\varepsilon_k = -2t(\cos k_x + \cos k_y) - 4U^2 \cos k_x \cos k_y$ is the dispersion with hopping $t$ and next-nearest-neighbor hopping $t'$. We define the single particle Green’s function as $G_{\sigma}(k_1 \tau_1, k_2 \tau_2) = (T_\tau(c_{k_1 \sigma}^\dagger c_{k_2 \sigma}))$ and the two-particle Green’s function as $G_{\sigma \sigma'}(k_1 \tau_1, ..., k_4 \tau_4) = (T_\tau(c_{k_1 \sigma}^\dagger c_{k_2 \sigma'} c_{k_3 \sigma'} c_{k_4 \sigma}))$, with conservation of momentum $k_1 + k_3 = k_2 + k_4$, and $\tau_i$ denote imaginary time points.

The generalized susceptibility is defined as
$$\chi_{\omega, \Omega}(k, k', q) = \int_0^\beta d\tau' \sum_{\kappa \kappa'} \delta \Gamma_{\kappa \kappa'}(k, \kappa', q) \delta G_{\kappa} \delta G_{\kappa'}(k), \quad (2)$$

with $\omega = \omega_0 q$ and $\Omega = \Omega_0 q$.

The “density channel” susceptibility is then defined as
$$\chi^\omega_d(k, k', q) = \chi^\omega_{ph}(k, k', q) + \chi^\omega_{p}(k, k', q), \quad (3)$$

and can be decomposed using Bethe Salpeter equation into
$$\chi^\omega_d(k, k', q) = \chi^\omega_d(k, k', q) - \frac{1}{\beta^2 N^2} \chi^\omega_{\Omega}(k, k, q) \chi^\omega_{\Omega}(k, k, q) \chi^\omega_d(k, k', q), \quad (4)$$

with $\chi^\omega_d(k, k', q) = -\beta N G_{\sigma}(i \omega, k) G_{\sigma}(i \omega + i \Omega, k + q) \delta G_{\delta(k', k, q)}$ the irreducible vertex in the density channel. $N$ denotes the number of $k$ points for the summation over $k_1, k_2, k_3, k_4$.

Linear response theory relates $\chi_d$ to a generating field $\Lambda(k)$ as
$$-\frac{1}{N_0} \int_0^\beta dr' \sum_{\kappa \kappa'} \delta G_{\kappa}(k, \kappa', q, 0, k, 0; \Lambda) \left. g(k) g(k') \right|_{\Lambda = 0} = \frac{1}{\beta^2 N_0} \sum_{\omega, \kappa \kappa'} \chi^\omega_d(k, k', q) g(k) g(k'). \quad (5)$$

Superconducting fluctuations are related to the susceptibility in the particle-particle channel which follows from an analogous derivation,

$$\frac{1}{N_0} \int_0^\beta dr' \sum_{\kappa \kappa'} \delta G_{\kappa}(k, 0; \eta) g(k) g(k') \left|_{\eta = 0} \right. = \frac{1}{\beta^2 N_0} \sum_{\omega, \kappa \kappa'} \chi^\omega_g(k, k', q = 0) g(k) g(k'). \quad (6)$$

with $F(k, \tau) = -\langle T_\tau c_{k,1}^\dagger c_{k-\tau,1}(0) \rangle$ the anomalous Green’s function, and $\eta(k)$ the generating field. The related order parameter is $P = \sum_k g(k) c_{k,1} c_{-k,1}$.

We define the right hand side quantity in both Eq(6) and Eq(5) as $\chi_g$,

$$\chi_g = 1 \frac{1}{\beta^2 N_0} \sum_{\omega, \kappa \kappa'} \chi^\omega_g(k, k', q) g(k) g(k'). \quad (7)$$

This is the central quantity investigated in this paper.

Phase transitions are indicated by a divergence of the susceptibility $\chi^\omega_{\Omega}(k, k', q)$ and Eq. (7) as $\chi_g$.

$$V_g := \langle \chi - \chi_0 \rangle_g = 1 \frac{1}{\beta^2 N_0} \sum_{\omega, \kappa \kappa'} g(k) g(k') \times (\chi^\omega_{\Omega}(k, k', q) - \chi^\omega_{\Omega}(k, k', q)) \quad (8)$$

in analogy to $P_g$ in the superconducting case. This quantity highlights vertex contributions by subtracting band-structure and single-particle effects contained within the bare susceptibility.

We will show that charge fluctuations with momentum transfer $q = (\pi, \pi)$ and d-wave symmetry are large. These fluctuations are known as d density wave. Ref. [70] defines density order in analogy with superconductivity, with a single order parameter in the form $\langle \psi_{k,1}^\dagger(k + q) \psi_{k,1}(0) \rangle = \Phi_0 f(k) \delta_{\kappa, \beta}$ for symmetry factor $f(k)$. Two of the possible orders are $f(k) = \sin k_x$ for $p_x$ symmetry and $f(k) = \cos k_x - \cos k_y$ for $d_{x^2-y^2}$ symmetry. d density wave, also called “staggered flux state”, occurs at $Q = (\pi, \pi)$. $p_x$ density wave (PDW), also called “bond order wave”, happens at $Q = (\pi, \pi)$ and $(\pi, 0)$.

The exact solution of the Hamiltonian, Eq. (1) is unknown. Here we use the dynamical cluster approximation (DCA), which approximates the self-energy by $N_c$ coarse-grained patches in which the self energy is momentum independent, but retains the full frequency dependence. The method is approximate but controlled in the sense that the thermodynamic limit for local quantities are approached as $N_c \to \infty$. The eight-site cluster used here is a compromise chosen large enough to accommodate a clear nodal-antinodal differentation pseudogap region, and superconductivity, while remaining cheap enough for simulation of a wide range of parameters.

Fig. 7 shows the phase diagram of the model obtained within the 8-site DCA with parameters $U/t = 7$.
and $t'/t = -0.15$. These parameters are chosen to represent the overall phase diagram common to several cuprate. The pseudogap regime is obtained by observing a suppression in the single-particle spectral function. The superconducting phase is computed in a Nambu formulation and defined as the area where the anomalous Green’s function $F(k, \tau) = -(T_{\tau} c_{k,\uparrow}(\tau)c_{-k,\downarrow}(0))$ at $k = (0, \pi), (\pi, 0)$ becomes nonzero.

DCA only yields the cluster Green’s functions and corresponding cluster susceptibilities $\chi_0^{\omega, d}(K, K', Q)$ at the cluster momenta $K, K'$ and $Q$. The corresponding approximation to Eq. 4 is obtained by interpolating $\chi_d(k, k', Q) = (\chi_0^{-1}(k, k', Q) + \chi_c^{-1}(K, K', Q) - \chi_0^{-1}(K, K', Q))^{-1}$. This is analogous to identifying the DCA cluster vertex with the lattice vertex $\Gamma^\pm_0=\Omega(k_1, k_2, q)$ [25].

Within the eight site cluster, the symmetry factors we used below corresponding to $s-, p_x, d_{xy}$ and $d_{x^2-y^2}$ symmetry are defined as $g_x(K) = 1$, $g_{p_y}(K) = \sin(K_x)$, $g_{d_{xy}}(K) = \sin(K_x)\sin(K_y)$, and $g_{d_{x^2-y^2}}(K) = \cos(K_x) - \cos(K_y)$. The DCA approximation generates strong antiferromagnetic (AFM) fluctuations with a correlation length comparable to the cluster size. If the establishment of long-range AFM order is allowed, the system chooses an ordered state at a temperature above the onset of the PG or superconductivity. This is a finite size effect [25]. For this reason, we suppress magnetic long-range order and only show results obtained in the paramagnetic state, which have the correlation length of AFM fluctuations restricted to the cluster size [25].

Our results are obtained with a continuous-time auxiliary field quantum Monte Carlo impurity solver [25,54] based on the ALP [25,55] libraries. The summation over fermionic frequencies in Eq. 4 and Eq. 8 goes over all frequencies from $-\infty$ to $\infty$. In our calculations, only a finite number of frequencies is available, but the asymptotic behavior of $\chi_0$ is known analytically [25]. In the results presented here, we use 36 fermionic frequencies for $\beta t = 5, 10$; 50 fermionic frequencies for $\beta t = 15, 20$; and 80 fermionic frequencies for $\beta t = 30$ on both positive and negative sides to compute the vertices. The relative change for omitting the last eight frequencies on each side is on the order of $10^{-3}$. The asymptotic behavior of vertex $\Gamma$ and $F$ is also analysed in Ref. [55] which provide an alternative way of treating the high frequency behavior. $\chi$ is computed with the number of frequencies listed above for the vertex correction part, plus $\chi_0$ computed with 1024 fermionic frequencies (both positive and negative) and supplemented with an analytically known asymptotic correction.

### III. CHARGE AND SUPERCONDUCTING FLUCTUATIONS

Fig. 2 shows six panels for the leading fluctuations at $\beta t = 20$ and $t'/t = -0.15$. The three rows represent $p_x$ and $d_{x^2-y^2}$ density fluctuations, and $d_{x^2-y^2}$ superconducting fluctuations. The left column shows $\chi_{d, \rho}$ (see Eq. 7), the right columns $|\chi - \chi_0|_2$ (see Eq. 8). Each panel displays data as a function of $U$ and doping $\delta$, with $\delta = 0$ corresponding to half filling. For superconductivity, only fluctuations with $d_{x^2-y^2}$ symmetry (DSC) are large [25]. Fig. 2(b), (d) and (f) illustrate that $\chi$ itself is not a good measure for the correlation contribution that may eventually drive the system to an ordered state, as most of $\chi$ stems from $\chi_0 = GG$. Fig. 2(e)-(f) show that the amplitude of DDW and DSC fluctuations are comparable (at the same order), implying competing fluctuations. However, we find numerically that DSC fluctuations are always larger than DDW for the parameters examined.
In a small regime of parameter space, where $U \sim 6.5t$ with slight electron doping, p-density wave fluctuations are the dominant charge fluctuation (panel (a) and (b)).

The maximum of DSC is on the electron doped side, while the maximum of DDW is on the hole doped side, both at intermediate interaction strength $U$. In addition, DSC fluctuations are suppressed in the pseudogap regime starting from $U \sim 6t$ (see Ref. 32 and 17), while DDW fluctuation start to show suppression around half filling for $U \sim 6.5t$, which corresponds to the onset of the Mott insulating state; its maximum is near $U \sim 6.5t$, which is the same interaction strength where DDW shows a suppression near half filling.

IV. TEMPERATURE EVOLUTION

In order to investigate the competition between d density wave and d wave superconducting fluctuations in more detail, we explore their temperature evolution with different dopings in Fig. 3. We show the results at $U = 7t$ and $t' = -0.15t$. Panel (b) shows that away from half filling, the vertex part of DSC increases as temperature decreases for all doping levels investigated (see also Ref. 32), whereas panel (a) shows that the vertex correction part of DDW increases as temperature decreases in the underdoped regime away from half filling but rapidly decays to zero for large doping. The maximum of the DSC fluctuations are near the maximum $t$, while the corresponding maximum DDW fluctuations occur at slightly lower doping. The transition to superconductivity on the hole doped side will take place near $\beta t = 35$ at optimal doping in this model, i.e. at a temperature about twice below where these results have been obtained.

The amplitude of the vertex correction part of DDW and DSC fluctuations as a function of temperature at the doping level corresponding to largest DDW fluctuation and largest DSC fluctuation is shown in Fig. 4. These results are obtained in the paramagnetic state but reach temperatures just above the superconducting transition. At the doping level where DDW fluctuations are strongest, DSC fluctuations are substantially larger than DDW, and increase faster as temperature decreases. We have been unable to find a region of parameter space where d density wave order prevails over superconductivity around optimal doping. At the doping level corresponding to largest DSC fluctuation we could find, DDW fluctuations first increase as temperature decreases, then start to decrease at $\beta t \sim 20$. This result is consistent with the findings of Ref. 77 and 91.

V. PARTICLE-HOLE ASYMMETRY

Fig. 5 shows the dependence of PDW and DDW on interaction and doping for three values of $t'$. $t'$ is to shift the Van Hove singularity of the density of states towards hole doping and destroys particle hole symmetry. We find that, as $t'/t$ is changed from 0 to $-0.2$ and correspondingly the Van Hove singularity more toward the hole doped side, PDW fluctuation spread out over a larger area of the parameter space at electron doped side, but their maximum does not change significantly. On the
other hand, the maximum of DDW fluctuation shift to-wards hole doping and their intensity decrease substan-tially. The particle hole asymmetry of DSC shows differ-ent trend as DDW. As \( t'/t \) increases, the maximum of DSC fluctuation moves to the electron-doped side. This is consistent with a scenario where the establishment of a pseudogap on the hole-doped side suppresses d-wave superconducting fluctuations.

Panel (a) of Fig. 6 shows the amplitude of the vertex corrections of DDW and DSC with different \( t' \) at \( U = 7t \), \( \beta t = 15 \), and doping levels corresponding to the largest DDW fluctuations. As \( t'/t \) increases, the maximum of DDW shifts toward the hole doped side. Since the over-all intensity of the fluctuations decreases, the maximum value of DDW fluctuations saturates and then drops. At the same time, for all the \( t' \) values we explore, DDW fluc-tuations are still weaker than DSC fluctuations around the optimal doping for DDW fluctuations. Panel (b) shows the doping levels where the largest DDW fluctuations are found.

8-site DCA shows a narrowing of the pseudogap on the electron doped side, and for \( t' < -0.15t \) has a first order transition between the Mott insulator and a momentum-dependent Fermi liquid state. This rapid change in the single-particle quantities does not show an analogue in the DDW or PDW fluctuations.

**VI. DISCUSSION**

The cause and consequence of DDW have been much debated. Early studies considered such fluctuations as a candidate for the mechanism of the pseudogap. Numerical calculations of the Hubbard model argued that this type of fluctuation is not strong enough to form an ordered state in the strongly correlated region, and is always dominated by DSC fluctuations. Other works have studied the coexistence of DDW and DSC order.

More recent VMC studies found staggered flux states (DDW states) in the strongly correlated under-doped regime of the Hubbard model, for interactions smaller than the Mott transition. They proposed this state as a candidate for an anomalous “normal state” competing with DSC since its properties are similar to those of the pseudogap. In these more recent works, the state does not coexist with DSC.

Our results clarify some of these arguments. Our interaction, doping and \( t' \) evolution of DDW correlations show that the evolution of the pseudogap and that of DDW correlations do not track each other. This can be seen from the fact that in the area around half fill-ing, where there is a pseudogap, DDW correlations show a suppression. However, the interaction strength where DDW starts to show a suppression is at \( U \sim 6.5t \), not at \( U \sim 6t \) where the pseudogap opens. As \( t' \) increases, the pseudogap regime moves to the hole doped side, while the suppression of DDW moves to the electron doped side. These trends show little overall correlation between areas with the largest DDW fluctuations and the appearance of a pseudogap.

Without entering an ordered phase, it is difficult to make statements about a potential coexistence of DDW and DSC. However, comparison between the temperature evolution of DDW and DSC at \( U = 7t \) (Fig. 3 and Fig. 1) clearly shows that around the optimal doping for DDW, DSC correlations are dominant over DDW and will order first. Thus, if there is a coexistence regime, it is likely fully contained inside the DSC dome.

Previous work investigated the competition between DSC and DDW in the Hubbard model with DCA on 4-site clusters at the two doping levels \( \delta = -0.05 \) and \( \delta = -0.25 \). The first doping level is in the pseudogap regime, the second far in the overdoped. The main finding, namely that the susceptibility corresponding to d density wave does not diverge, indicating the absence of a possible transition to the DDW state, is reproduced by our calculations. However, the claim that both DDW and DSC correlation functions are enhanced in the pseudo-gap regime is inconsistent with our more detailed calculations. The reason is that the intermediate maximum, which we find around \( \delta = -0.09 \), is missed by the coarse doping resolution employed in Ref.

Fluctuation diagnostic attributes contributions to the self-energy to fluctuations of different types. Ref. shows that in the parameter regime we explore in this paper, the dominant fluctuation in the normal state is always magnetic. It is shown in Ref. that these magnetic fluctuations are responsible for the major contribution to the single-particle self-energy, and thereby for the suppression of the density of states. The pseudogap in the Hubbard model can therefore clearly be attributed to magnetic fluctuations. DDW and DSC fluctuations do not directly contribute to a single particle self-energy, since the summation of a fluctuation with a d-wave symmetry tends to cancel out in the calculation of the self-energy.

The DCA simulations performed here are insensitive to the stripe order widely found in experiment and in numerical ground-state calculations. In order to find a transition to an ordered state in DCA, the ordering vector
VII. CONCLUSIONS

In conclusion, we have investigated the physics of short-range charge fluctuations in the strongly correlated regime of the 2D Hubbard model within the 8-site DCA approximation. We have found that the dominant charge fluctuations have d-wave symmetry, apart from a small regime near the Mott transition where we find p-wave charge fluctuation. For all doping, interaction, and next-nearest hopping parameters investigated, we showed that superconducting d-wave fluctuation are always stronger than charge fluctuations away from half filling. At $U = 7t$, at the doping level that is most favorable for DDW, DSC will order first as temperature decreases, showing that if there was a coexistence of DDW and DSC orders, the coexistence area would likely be fully contained inside the DSC dome.

Our parameter scans show that DDW fluctuation cannot be viewed as the cause of the pseudogap in the single-particle density of states, as the change of DDW fluctuations does not match the evolution of the pseudogap. This is consistent with the results of several recent works, including Refs. [53,54] that show convincingly that the pseudogap can be attributed to strong short-wavelength AFM correlations.

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