Bond excitations in the pseudogap phase of the Hubbard Model

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Using the dynamical cluster approximation, we calculate the correlation functions associated with the nearest neighbor bond operator which measure the z component of the spin exchange in the two-dimensional Hubbard model with $U$ equal to the bandwidth. We find that in the pseudogap region, the local bond susceptibility diverges at $T = 0$. This shows the existence of degenerate bond spin excitation and implies quantum criticality and bond order formation when long range correlations are considered. The strong correlation between excitations on parallel neighboring bonds suggests bond singlet dimerization. The suppression of divergence for $n < \approx 0.78$ implies that for these model parameters this is quantum critical point which separates the unconventional pseudogap region characterized by bond order from a conventional Fermi liquid.

Introduction. The low doping pseudogap (PG) region of the cuprates has remained an issue of great discussion and controversy, with experimental data showing anomalous behavior such as the suppression of spin excitations in the susceptibility, a PG in the single-particle spectra, and patterns in the STM spectra, among others. Different investigators argued that the PG is related with the settlement of long range order at a general phase transition. Nevertheless, in the limit $N_c \to \infty$ one should expect that long range bond correlations will quench the entropy and a transition to a state with long range order will take place, unless a stronger instability such as d-wave pairing occurs first. The DCA method, which does not allow spatial ordering on distances larger than the cluster size, will fail to capture this transition when small clusters are considered. However at temperatures larger than the ordering temperature the physics would be determined predominantly by the local quantum fluctuations described with DCA. The divergent behavior of bond susceptibility is suppressed for doping $> 22\%$ implying that for these model parameters, $22\%$ doping is a QCP which separates the unconventional pseudogap region characterized by bond order from a conventional Fermi liquid. We also find a strong correlation between excitations on parallel neighboring bonds, which suggests that the pseudogap region is characterized by bond singlet dimerization.

Formalism. To solve the cluster problem we use the Hirsch-Fye quantum Monte Carlo (QMC) method which is based on a discrete path integral approximation with time step $\Delta \tau$. Hirsch-Hubbard-Stratonovich (HHS) fields are introduced to decouple the interaction:

$$
\exp(-\Delta \tau U n_\uparrow n_\downarrow + \Delta \tau U (n_\uparrow + n_\downarrow)/2) = \frac{1}{2 \text{Tr} \sigma^2 \sigma (n_\uparrow - n_\downarrow)}.
$$

(1)

where an Ising HHS decoupling field $\sigma = \pm 1$ is introduced at each spin-time location on the cluster. This transforms the problem of interacting electrons to one of non-interacting particles coupled to time-dependent fields. The fermionic fields are then integrated out, and the integrals over the HHS decoupling fields are performed with a Monte Carlo algorithm.

All measurable quantities are completely determined
by the HHS fields and the host Green’s function. The HHS fields contain all information about correlations (spin, pair and charge) in space and time. Moreover, Hirsch has shown that spin correlations may be directly rewritten in terms of the HHS decoupling fields\[16, 17\]. One may interpret the Ising fields as representing the fermion spin variables

\[\langle n(i, \tau) - n(i, \tau) \rangle \rightarrow \left(1 - e^{-\Delta T U}\right)^{-1/2} \sigma(i, \tau).\]  

Note that this is an exact mapping, so that all correlation functions of the HHS fields are, up to a proportionality constant, equivalent to the corresponding correlation functions of \(S^z(i, \tau) = \frac{1}{2} \langle n(i, \tau) - n(i, \tau) \rangle\).

In the DCA the single-particle and two-particle lattice response functions are calculated with the Dyson equation using the irreducible cluster self-energy and vertices, respectively. Unlike experiments, where in order to search for quantum criticality, a magnetic field is applied to suppress the superconductivity, in DCA the superconductivity can be suppressed by imposing a normal state host. We then look for divergent susceptibilities in the normal state indicating phase boundaries. Lattice two-particle susceptibilities indicate transitions to antiferromagnetic (AF) and d-wave superconducting states at finite doping according to the phase diagram shown in Fig. 1. However ordering associated with more complex operators, such as valence bond singlets\[16\], is far more difficult to detect with the DCA, since it involves complex equations and up to eight-leg irreducible interaction vertices. More feasible calculations involve the corresponding cluster susceptibilities, since they can be obtained directly in the QMC process. However, these cluster susceptibilities are finite size quantities and can diverge only at zero temperature (i.e., infinite imaginary time when ordering in time occurs).

To study bond correlations, we define the bond "ij" operator at time \(\tau\) as

\[B(i, j; \tau) = \sigma(i, \tau)\sigma(j, \tau) \propto S^z(i, \tau)S^z(j, \tau)\]  

where "i" and "j" label the position in the cluster. For simplicity, we also denote with \(B_{nn}(B_{nnn})\) the bond operator when "i" and "j" are (next) nearest neighbor sites.

In the next section we present results for the correlation functions:

\[\chi_0(T) = \int d\tau \langle \delta B(i; i + \hat{x}, \tau)\delta B(i; i + \hat{x}, 0)\rangle\]  
\[\chi_\perp(T) = \int d\tau \langle \delta B(i; i + \hat{x}, \tau)\delta B(i; i + \hat{y}, 0)\rangle\]  
\[\chi_\parallel(T) = \int d\tau \langle \delta B(i; i + \hat{x}, \tau)\delta B(i; i + \hat{x} + \hat{y}, 0)\rangle\]  

where

\[\delta B(i; i + \hat{x}, \tau) = B(i; i + \hat{x}, \tau) - \langle B_{nn}\rangle.\]

We also measure \(\chi_\sigma\), the susceptibility associated with the operator \(M\)

\[M(\tau) = \frac{1}{N} \sum_{ij} \left(B(i, i + \hat{x}; \tau) + B(i, i + \hat{y}; \tau)\right)\]  
\[\chi_\sigma(T) = \int d\tau \langle \delta M(\tau)\delta M(0)\rangle.\]

These correlation functions describe the response of the system to an external field which couples with the bond operator \(B_{nn}\). The field acts to modify the z-component of the nearest neighbor exchange interaction. Depending on its sign it decreases or increases the energy of an AF bond and has an opposite effect on a FM bond. \(\chi_0\) describes the local bond response while \(\chi_\perp\) and \(\chi_\parallel\) the correlation between nearest neighbor bonds. \(\chi_\sigma\) is a cluster quantity incorporating spatial correlations within the cluster between bonds.

Results. We first present calculations on a 2 × 2 cluster, the smallest cluster capable of reproducing the generic features of the cuprate phase diagram. In the doping region relevant for high Tc cuprates, the Hubbard model shows evidence of short range AF correlations. The expectation value of (next) nearest neighbor bond operator \(B_{nn}(B_{nnn})\) is negative (positive) and increases with lowering temperature, as one expects for a system with short range AF order. The short range AF order is stronger at smaller doping. \(B_{nn}\) and \(B_{nnn}\) versus temperature at different fillings are shown for a \(N_z = 4\) cluster in Fig. 2-a) and, respectively, -b).

In the electron density range \(1 > n > \sim 0.78\), the temperature dependence of the local bond susceptibility shows the existence of degenerate or almost degenerate states with different magnitude of their bond value \(B_{nn}\). This doping range roughly corresponds to the pseudogap region of an \(N_z = 4\) cluster, see Fig. 1. As shown in Fig. 2-c) the extrapolation of our data indicate that \(\chi_0\) is diverging when \(T \rightarrow 0\). Since the lowest temperature we can reach is \(\approx 0.01t\) the apparent divergent \(\chi_0\) implies, if
not degenerate states, at least bond excitations with an energy much smaller than this scale.

In the pseudogap region (i.e., $1 > n > \sim 0.78$) $\chi_0$ diverges as $\sim \frac{1}{T}$. This can be seen in Fig. 3-a) where we show (black line) $T\chi_0$ versus $T$ at filling $n = 0.88$. $T\chi_0$ displays a linear behavior and, at $T = 0$, extrapolates to a finite value, albeit small, $\mu_0^2$. The $\sim \frac{1}{T}$ dependence of susceptibility is consistent with scenarios which assume two degenerate configurations, 1 and 2, with different bond values such that $2\mu_0 = B_{nn}(1) - B_{nn}(2)$. It is instructive to draw an analogy with local spin susceptibility of a system with independent local moments. A free moment is a doubly degenerate problem where the spin can be aligned parallel or antiparallel to a particular direction. A perturbing magnetic field lifts the degeneracy of the two configuration by an amount proportional to the moment and the magnetic field. Similarly, in our system the perturbing Hamiltonian acting on the bond $(ij)$, $H^{ext} = hB(i,j)$, splits the configurations with an amount proportional to the field $h$ and $B(i,j)(1) - B(i,j)(2)$. Thus, the $\sim \frac{1}{T}$ dependence of the local bond susceptibility suggests the existence of two degenerate states with different bond magnitude. Of course other scenarios compatible with a $\sim \frac{1}{T}$ like susceptibility cannot be excluded.

The bond correlations are strongest around $n \approx 0.88$ and weak at small and large doping. This can be seen both by inspecting $\chi_0(T)$ in Fig. 2-c) and by looking at the bond moment $\mu_0^2$ versus filling in Fig. 3-b). At half filling, the bond moment extrapolates to zero, since the numerical data does not show evidence of divergent susceptibilities in the undoped system. At finite doping $\mu_0^2$ increases with increasing doping displaying a maximum at $n \approx 0.88$. $\mu_0^2(n)$ decreases with further doping until it vanishes at $n \approx 0.78$.

At low temperatures we find a strong positive correlation between nearest neighbor parallel bonds and a small negative correlation between nearest neighbor perpendicular bonds. This is shown in Fig. 4-c). $\chi_{\parallel}$ is increasing strongly with lowering $T$, the numerical data indicating even a possible divergence when $T \to 0$, although weaker than $\sim \frac{1}{T}$ characteristic to local bond fluctuations (see Fig. 3-a). The large value of $\chi_{\parallel}$ shows that increasing or reducing the antiferromagnetism on a bond implies a similar effect on the nearest neighbor parallel bond. Whereas the correlation between nearest neighbor perpendicular bond fluctuations $\chi_{\perp}$ is much smaller and negative. Larger cluster calculations are limited to finite tem-
temperatures due to the minus-sign problem present in the Hirsch-Fye algorithm. For example, for the values of $U/W$ used here, when $N_c = 16$ the minus sign limits Hirsch-Fye QMC calculations to $4t/\beta \leq 36$ for fillings in the pseudogap region. Down to this temperature the local bond correlation $\chi_0(T)$ looks similar to the one calculated for $N_c = 4$, but this temperature is too large for a reliable extrapolation to $T = 0$. However, by increasing the cluster size and thus incorporating spatial correlations at larger length scale one expects a decrease of $\mu_0$ or even the disappearance of the divergent behavior due to the settlement of bond order. This is similar to the disappearance of the $T = 0$ divergence in the local spin susceptibility when going from an atom to finite cluster due to the settlement of short range AF order.

In order to investigate critical fluctuations as a function of the cluster size we calculate the cluster bond correlation $\chi_s(T)$ defined in Eq. 9. While the zero temperature divergence of $\chi_0(T)$ is suppressed in larger clusters due to correlations between the bonds, $\chi_s(T)$ would still be divergent provided that short ranged order between the bonds emerges. The plots in Fig. 4-a) of $\chi_s(T)$ for $N_c = 2$, $N_c = 4$ and $N_c = 16$ at $n = 0.88$ indicate that unquenched bond fluctuations persists with increasing cluster size. For $N_c = 2$ (black), $\chi_s(T)$, which in this case coincides with the local bond $\chi_0(T)$, does not show divergent behavior at zero temperature. $\chi_s(T)$ for $N_c = 4$ diverges at $T = 0$ since it contains the divergent $\chi_0(T)$ term. For $N_c = 16$ and at the accessible temperatures, $\chi_s(T)$ increases more strongly with decreasing temperature than for the $N_c = 4$ case, thus showing an even more divergent behavior. Of course, the large value of $\chi_s$ for $N_c = 16$ show the importance of spatial correlations between bond fluctuations. As for the $N_c = 4$ cluster, we find that for $N_c = 16$ the correlations between nearest neighbor parallel bonds is more important than the correlations between nearest neighbor perpendicular bonds, as the difference between $\chi_\parallel$ and $\chi_\perp$ plotted in Fig. 4-c shows.

Notice that even for the $N_c = 16$ cluster the divergent behavior of $\chi_s(T)$ ceases when $n \approx 0.78$ as can be seen in of Fig. 4-b, indicating that $n \approx 0.78$ is a QCP. The smaller (larger) doping region would presumably correspond to a state with (without) bond order when $N_c \to \infty$.

Discussion

Without dismissing other possibilities, we note that a scenario where the system forms adjacent parallel bond singlets fits very well with our results. For instance the divergence of local bond susceptibility $\chi_0$ requires two degenerate states with different $B_{mn}$. Suppose we measure $\chi_0$ on a bond along $x$ direction. A configuration with adjacent parallel bond singlets along $x$, such as one in Fig. 5-a), has a $B_{mn} = -1$, while a configuration with adjacent parallel bond singlets along $y$, such as one in Fig. 5-b), has a $B_{mn} = 0$. If these two configurations are degenerate they will yield a divergent $\chi_0$. Moreover the correlation between parallel bond excitations will be also divergent and positive, while the correlation between nearest neighbor perpendicular bonds will be negative, resembling our findings on the $2 \times 2$ cluster.

Conclusions

The behavior of bond susceptibility in the PG region of the 2D Hubbard model calculated with DCA shows evidence of quantum criticality and implies settlement of bond order. Thus, in the the $2 \times 2$ cluster we find divergent local bond susceptibility at $T = 0$, which implies ordering in the imaginary time due to the existence of degenerate bond spin excitations. We find a strong correlation between excitations on parallel neighboring bonds, which suggests that the pseudogap region is characterized by bond singlet dimerization. We argue that the existence of unquenched local zero energy fluctuations for small $N_c$ implies long range order in the limit $N_c \to \infty$ or the intervention of competing phase transition. The suppression of divergence for $n \approx 0.78$ implies that $n \approx 0.78$ is a QCP which separates the unconventional pseudogap region characterized by dimers from a conventional Fermi liquid.

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