d-wave Superconductivity in the Hubbard Model

Th. Maier, M. Jarrell, Th. Pruschke, J. Keller

1 Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg
2 Department of Physics, University of Cincinnati, Cincinnati, OH 45221-0011

(October 29, 2018)

The superconducting instabilities of the doped repulsive 2D Hubbard model are studied in the intermediate to strong coupling regime with help of the Dynamical Cluster Approximation (DCA). To solve the effective cluster problem we employ an extended Non Crossing Approximation (NCA), which allows for a transition to the broken symmetry state. At sufficiently low temperatures we find stable d-wave solutions with off-diagonal long range order. The maximal $T_c \approx 150K$ occurs for a doping $\delta \approx 20\%$ and the doping dependence of the transition temperatures agrees well with the generic high-$T_c$ phase diagram.

Introduction  The discovery of high-$T_c$ superconductors has stimulated strong experimental and theoretical interest in the field of strongly correlated electron systems. After a decade of intensive studies we are still far from a complete understanding of the rich physics observed in high-$T_c$ cuprates. Angle resolved photoemission experiments on doped materials show a $d$-wave anisotropy of the pseudogap in the superconducting state. In underdoped materials even in the normal state this pseudogap persists, which is believed to cause the unusual non-Fermi-liquid behavior in the normal state. This emphasizes the importance of achieving a better understanding of the superconducting phase, i.e. the physical origin of the pairing mechanism, the nature of the pairing state and the character of low energy excitations.

On a phenomenological basis the $d$-wave normal state pseudogap as well as the transition to a superconducting state with a $d$-wave order parameter has been described within theories where short-ranged antiferromagnetic spin fluctuations mediate pairing in the cuprates.

On a microscopic level it is believed that the Hubbard model or closely related models like the t-J model should capture the essential physics of the high-$T_c$ cuprates. However, despite years of intensive studies, these models remain unsolved except in one or infinite dimensions.

Finite size QMC calculations for the doped 2D Hubbard model in the intermediate coupling regime with Coulomb repulsion $U$ less than or equal to the bandwidth $W$, support the idea of a spin fluctuation driven interaction mediating $d$-wave superconductivity. But the fermion sign problem limits these calculations to temperatures too high to observe a possible Kosterlitz-Thouless transition for the 2D system. Another problem encountered in QMC calculations is their finite size character, which makes statements for the thermodynamic limit dependent on a scaling ansatz.

These limitations do not apply to approximate many particle methods like the Fluctuation Exchange Approximation (FLEX). Results of FLEX calculations for the Hubbard model are in agreement with QMC results, i.e. they show evidence for a superconducting state with $d$-wave order parameter at moderate doping for sufficiently low temperatures. But the FLEX method as an approximation based on a perturbative expansion in $U$ breaks down in the strong coupling regime $U > W$, where $W$ is the bare bandwidth. On the other hand it is believed that a proper description of the high-$T_c$ cuprates in terms of the one-band Hubbard model requires $U > W$.

Calculations within the Dynamical Mean Field Approximation (DMFA) can be performed in the strong coupling regime and take place in the thermodynamic limit. But the lack of non-local correlations inhibits a transition to a state with a non-local ($d$-wave) order parameter. The recently developed Dynamical Cluster Approximation (DCA) is a fully causal approach which systematically incorporates non-local corrections to the DMFA by mapping the lattice problem onto an embedded periodic cluster of size $N_c$. For $N_c = 1$ the DCA is equivalent to the DMFA and by increasing the cluster size $N_c$, the dynamic correlation length can be gradually increased while the DCA solution remains in the thermodynamic limit.

Using a Nambu-Gorkov representation of the DCA we observe a transition to a superconducting phase in doped systems at sufficiently low temperatures. This occurs in the intermediate to strong coupling regime $U > W$ and the corresponding order parameter has $d$-wave symmetry.

Method  A detailed discussion of the DCA formalism was given in previous publications where it was shown to systematically restore momentum conservation at internal diagrammatic vertices which is relinquished by the DMFA. However, the DCA also has a simple physical interpretation based on the observation that the self-energy is only weakly momentum dependent for systems where the dynamical intersite correlations have only short spatial range. The corresponding self-energy is a functional of the interaction $U$ and the Green function propagators. The latter may be calculated on a coarse grid of $N_c = L^D$ selected K-points only, where $L$ is the...
linear dimension of the cluster of $K$-points. According

to Nyquist’s sampling theorem [14], this sampling of the

reciprocal space at intervals of $\Delta K = 2\pi/L$ implies that

the DCA incorporates nonlocal dynamical correlations

with a spatial range $L/2$ and cuts off longer ranged

dynamical correlations. Knowledge of the momentum

dependence on a finer grid may be discarded to reduce

the complexity of the problem. To this end the first Brillouin

zone is divided into $N_c$ cells of size $(2\pi/L)^D$ around

the cluster momenta $K$ (see Fig.1). The Green functions

used to form the self-energy $\Sigma(k,\omega)$ are coarse grained,

or averaged over the momenta $K + k$ surrounding the

cluster momentum points $K$ (cf. Fig.1).

Thus, the coarse grained Green function is

$$\hat{G}(K,\omega) = \frac{N_c}{N} \sum_k \hat{G}(K + k,\omega),$$

(1)

where the sum runs over all vectors $k = K + k$ within

a cell around the cluster momentum $K$. Note that the

choice of the coarse grained Green function has two well

defined limits: For $N_c = 1$ the sum over $k$ runs over the

entire Brillouin zone, $\hat{G}$ is the local Green function, thus

the DMFA algorithm is recovered. For $N_c = \infty$ the $k$-

summation vanishes and the DCA becomes equivalent to

the exact solution. The dressed lattice Green function

takes the form

$$\hat{G}(K,\omega) = \left(\omega \mathbb{1} - \hat{e}_K \tau_3 - \hat{\Sigma}(K,\omega)\right)^{-1},$$

(2)

with the self-energy $\hat{\Sigma}(k,\omega)$ approximated by the clus-
ter self-energy $\hat{\Sigma}(K,\omega)$. To allow for a possible transi-
tion to the superconducting state we utilized the Nambu-
Gorkov matrix representation [15] in (2) where the self-
energy matrix $\hat{\Sigma}$ is most generally written as an expan-
sion $\hat{\Sigma} = \sum_{i} \Sigma_i \tau_i$ in terms of the Pauli matrices $\tau_i$. The

diagonal components of $\hat{\Sigma}$ represent quasiparticle renor-
malizations, whereas the offdiagonal parts are nonzero in

the superconducting state only.

Since the self-energy $\hat{\Sigma}(K,\omega)$ does not depend on the

integration variable $k$, we can write

$$\hat{G}(K,\omega) = \left(\omega \mathbb{1} - \hat{e}_K \tau_3 - \hat{\Sigma}(K,\omega) - \hat{\Gamma}(K,\omega)\right)^{-1},$$

(3)

where $\hat{e}_K = N_c/N \sum_k \epsilon_{K + k}$. This has the form of the

Green function of a cluster model with periodic boundary

conditions coupled to a dynamic host described by

$\hat{\Gamma}(K,\omega)$. Here we employ the NCA to calculate the clus-
ter Green function and self-energy respectively. A de-
tailed discussion of the NCA-algorithm applied to the

cluster model for the paramagnetic state was given in

[12]. The NCA for the superconducting state has to be

extended in order to account for the hybridization to the

anomalous host, which couples cluster states with differ-

cent particle numbers.

The self-consistent iteration is initialized by calculating

the coarse grained average $\hat{G}(K)$ (Eq. 1) and with Eq.

3 the host function $\hat{\Gamma}(K)$, which is used as input for the

NCA. The NCA result for the cluster self-energy $\hat{\Sigma}(K)$

is then used to calculate a new estimate for the coarse

grained average $\hat{G}(K)$ (Eq. 1). The procedure continues

till the self-energy converges to the desired accuracy.

**Results**

We investigate the single particle properties of the doped 2D Hubbard Model

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(4)

where $c_{i\sigma}^\dagger$ (c$_i$) creates (destroys) an electron at site $i$ with

spin $\sigma$ and $U$ is the on-site Coulomb repulsion. For the

Fourier transform of the hopping integral $t_{ij}$ we use

$$\epsilon_k = \epsilon_0 - \mu - 2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y,$

(5)

accounting for both, nearest neighbor hopping $t$ and next

nearest neighbor hopping $t'$. We set $t = 0.25 eV$ and

$U = 3 eV$, well above the bandwidth $W = 8t = 2 eV$. For

this choice of parameters the system is a Mott-Hubbard

insulator at half filling as required for a proper descrip-

tion of the high-$T_c$ cuprates.

To allow for symmetry breaking we start the iteration

procedure with finite offdiagonal parts of the self-energy

matrix $\hat{\Sigma}$. As we mentioned above one expects the order

parameter of a possible superconducting phase to have

$d$-wave symmetry. Therefore we work with a 2x2-cluster

($N_c = 4$), the smallest cluster size incorporating nearest

neighbor correlations. For the set of cluster points we

choose $K_{m\ell} = l \pi$, where $\ell = 0,1$ and $\alpha = x$ or $y$. Fig.1

illustrates this choice of $K$-points along with a sketch of

the $d$-wave order parameter and the coarse graining

cells. Obviously, for symmetry reasons, in the case of

$d$-wave superconductivity, we expect the coarse grained

anomalous Green function to vanish at the zone center.
and the point $(\pi, \pi)$. Whereas the anomalous parts at the points $(0, \pi)$ and $(\pi, 0)$ should be finite with opposite signs.

The nearest neighbor hopping integral $t$ and the point $(\pi, \pi)$, and $K = (0, 0)$ and $K = (\pi, \pi)$). Thus a possible parameter. Note that this result is independent of the doping. However the drop in the density of states at the Fermi energy do not depend strongly upon doping. However the drop in the gap size, measured as the peak to peak distance, as well as the density of states at the Fermi energy do not depend strongly upon doping. However the drop in the density of states from the gap edge to the $\omega = 0$ value first increases, reaches a maximum at about 19% doping, then decreases again.

FIG. 2. (a) The local density of states (DOS) near the Fermi energy and the anomalous coarse grained Green functions at the cluster points (b) $K = (0, 0)$ and $K = (\pi, \pi)$, (c) $K = (\pi, 0)$ and (d) $K = (0, \pi)$ in the superconducting state. The nearest neighbor hopping integral $t = 0.25$eV, next nearest neighbor hopping integral $t' = 0$, bandwidth $W = 2$eV, the on-site Coulomb repulsion $U = 3$eV, temperature $T = 137$K and the doping $\delta = 0.19$. The anomalous parts of the Green function (b)-(d) are consistent with a $d$-wave order parameter.

Fig. 2 shows a typical result for the local density of states (DOS) in the superconducting state along with the anomalous coarse grained Green function $G_{12}(K, \omega) = N_c/N \sum_k \langle \langle c_{k+\delta\tau} c_{-(K+\delta\tau)} \rangle \rangle \omega$ at the cluster $K$-points for $t' = 0$, temperature $T = 137$K and doping $\delta = 0.19$. The anomalous coarse grained Green function vanishes at the cluster points $(0, 0)$ and $(\pi, \pi)$ but is finite at the points $(\pi, 0)$ and $(0, \pi)$, consistent with a $d$-wave order parameter. Note that this result is independent of the initialization of the self-energy, i.e. an additional initial $s$-wave contribution vanishes in the course of the iteration. Thus a possible $s$-wave contribution to the order parameter can be ruled out.

The finite pair amplitude is also reflected in the local density of states (DOS) depicted in Fig. 2a, where we show the lower sub-band of the full spectrum near the Fermi energy. It displays a pseudogap at zero frequency as expected for a $d$-wave order parameter.

Fig. 2 shows the DOS near the Fermi energy for the same parameters as in Fig. 2 fixed temperature $T = 137$K, but for various dopings. Obviously, the pseudogap size, measured as the peak to peak distance, as well as the density of states at the Fermi energy do not depend strongly upon doping. However the drop in the density of states changes from the gap edge to the $\omega = 0$ value first increases, reaches a maximum at about 19% doping, then decreases again.

FIG. 3. Density of states in a narrow region at the Fermi energy for the same parameters as in Fig. 2 but for various dopings. The gap size and the density of states at $\omega = 0$ are independent of doping. Inset: Equal time coarse grained anomalous Green function $G_{12}(K, \tau = 0)$ at $K = (\pi, 0)$.

This behavior originates in the doping dependence of the anomalous Green function. In the inset we plot the coarse grained anomalous equal time Green function $G_{12}(K, \tau = 0) = N_c/N \sum_k \langle \langle c_{k+\delta\tau} c_{-(K+\delta\tau)} \rangle \rangle$ for $K = (\pi, 0)$. This number as a measure of the superconducting gap shows exactly the same behavior as the pseudogap in the density of states.

The anomalous components $G_{12}(K, \omega)$ and hence the pseudogap in the DOS become smaller with increasing temperature and eventually vanish at a critical temperature $T_c$ depending on the set of parameters. The phase diagram is shown in Fig. 3. As a function of doping, $T_c(\delta)$ has a maximum $T_c^{\max} \approx 150$K at $\delta \approx 19\%$ and strongly decreases with decreasing or increasing $\delta$. The qualitative behavior of $T_c(\delta)$ in the calculated $T - \delta$ region agrees well with the generic phase diagram of the high-$T_c$ cuprates. Unfortunately, due to the break-down of the NCA at very low temperatures we are not able to extend the phase diagram beyond the region shown in Fig. 3. This means in particular that we cannot predict reliable values for $\delta_c(T = 0)$, beyond which superconductivity vanishes.

The inset of Fig. 3 shows the transition temperature dependence $T_c(t', \delta = \text{const.})$ on the next nearest neighbor hopping amplitude $t'$ for fixed doping $\delta = 0.18$. As compared to $t' = 0 T_c$ strongly decreases with growing negative $t'$ but increases for $t' > 0$. The shape of the phase diagram as well as the $t'$-dependence of $T_c$ can be qualitatively understood in terms of the phenomenological picture, where spin fluctuations mediate the electron-electron interaction, which then is strong at the antifer-
romagnetic wave vector $\mathbf{Q} = (\pi, \pi)$.

In Fig. 4 we display the coarse grained spectra $-\frac{1}{2} \delta m \tilde{G}_{11}(\mathbf{K}, \omega)$ at $\mathbf{K} = (\pi, 0)$ in the normal state ($T = 290 K$) for the next nearest neighbor hopping $t' = 0$ and $t' = -0.05 eV$ (left and right hand side) for different dopings $\delta$. At the bottom we show the Fermi surfaces of the corresponding noninteracting systems ($U = 0$) in the first quadrant of the BZ. The diagonal thick solid line indicates the set of $k$-points which fulfill the nesting condition, i.e. which can be connected by $\mathbf{Q}$ to equivalent $k$-points in the opposite quadrant of the BZ.

The doping dependence of the $t' = 0$ and $t' = -0.05 eV$ spectra is qualitatively different. In the $t' = -0.05 eV$ case the parts of the Fermi surface near $\mathbf{K} = (\pi, 0)$ and $(0, \pi)$ fulfill the nesting condition roughly for the whole doping range, the quasiparticles couple strongly to the spin fluctuations and hence the corresponding spectra display a pseudogap at zero frequency over the entire doping range. The $t' = 0$ spectra in contrast exhibit the pseudogap in the underdoped regime only ($\delta = 0.05$), where the spin fluctuations are strong, but show a quasiparticle peak at optimal doping $\delta = 0.19$, where the points on the Fermi surface near $\mathbf{K} = (\pi, 0)$ and $(0, \pi)$ are far from being nested. The suppression of the density of states at the Fermi energy results in a suppression of superconductivity and hence the transition temperatures drop with decreasing doping as well as decreasing $t' < 0$. For positive $t'$ we obtain similar spectra and Fermi surfaces as for $t' = 0$, but with a slightly enhanced density of states at the Fermi energy, resulting in higher transition temperatures.

**Summary** We have used the recently developed DCA to study the long open question of whether the 2D Hubbard model shows instabilities towards a superconducting state in the intermediate to strong coupling regime. We find conclusive evidence that at moderate doping a transition to a state with offdiagonal long range order occurs and that the corresponding order parameter has pure $d$-wave symmetry. The corresponding temperature-doping phase diagram agrees qualitatively with the generic high-$T_c$ phase diagram.

**Acknowledgements** It is a pleasure to acknowledge useful discussions with P.G.J. van Dongen, M. Hettler and H.R. Krishnamurthy. This work was supported by NSF grants DMR-9704021, DMR-9357199 and the Graduiertenkolleg “Komplexität in Festkörpern”. Computer support was provided by the Ohio Supercomputer Center and the Leibnitz-Rechenzentrum, Munich.

[1] For a review, see M.B. Maple, cond-mat/980202.
[2] H. Ding et al., Nature 382, 51 (1996).
[3] F. Ronning et al., Science (1998).
[4] For a review, see D.J. Scalapino, cond-mat/9908287.
[5] P. Monthoux, A.V. Balatsky and D. Pines, Phys. Rev. Lett., 67, 3448, (1991).
[6] T. Timusk and B. Statt, cond-mat/9905219.
[7] P.W. Anderson, The Theory of Superconductivity in the High-\textit{T}_c Cuprates, Princeton University Press, Princeton, NJ (1997).
[8] N.E. Bickers, D.J. Scalapino, and S.R. White, Phys. Rev. Lett., 62, 961 (1989).
[9] T. Moriya, Y. Takahashi, and K. Ueda, J. Phys. Soc. Japan, 59, 2905, (1990).
[10] W. Metzner and D. Vollhardt, Phys. Rev. Lett. 62, 324 (1989).
[11] M.H. Hettler \textit{et al}., Phys. Rev. B 58, 7475 (1998). M.H. Hettler \textit{et al}., preprint cond-mat/9903273.
[12] Th. Maier \textit{et al}., Eur. Phys. J. B 13, 613 (2000).
[13] C. Huscroft et al.,\textit{ cond-mat/9910226}.
[14] D.F. Elliot and K.R. Rao, Fast Transforms: Algorithms, Analyses, Applications (Academic Press, New York, 1982).
[15] J.R. Schrieffer, Theory of Superconductivity, Addison Wesley, Reading, MA (1993).
[16] H. Keiter, J.C. Kimball, Intern. J. Magnetism, 1, 233 (1971).