d-Wave Superconductivity in the Hubbard Model

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The superconducting instabilities of the doped repulsive 2D Hubbard model are studied in the intermediate to strong coupling regime with the help of the dynamical cluster approximation. To solve the effective cluster problem we employ an extended noncrossing approximation, 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 $T_c \approx 150$ K 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.

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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 [1]. Angle resolved photoemission experiments on doped materials show a d-wave anisotropy of the gap in the superconducting state [2]. In underdoped materials even in the normal state this pseudogap persists [2,3], 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 [4–6].

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 [7]. However, despite years of intensive studies, these models remain unsolved except in one or infinite dimensions.

Finite size quantum Monte Carlo (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 [4]. But the fermion sign problem limits these calculations to temperatures too high to observe a possible Kosterlitz-Thouless transition [4].

These limitations do not apply to approximate many particle methods like the fluctuation exchange approximation (FLEX) [8,9]. 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 [8,9]. 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 $U > W$, necessary for the experimentally observed Mott-Hubbard insulator at half filling.

Calculations within the dynamical mean field approximation (DMFA) [10] can be performed in the strong coupling regime and take place in the thermodynamic limit. But the lack of nonlocal correlations inhibits a transition to a state with a nonlocal (d-wave) order parameter. The recently developed dynamical cluster approximation (DCA) [11–13] is a fully causal approach which systematically incorporates nonlocal 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 [11–13] 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 $\mathbf{K}$ points only, where L is the linear dimension of the cluster of $\mathbf{K}$ points. 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 $\mathbf{K}$ (see Fig. 1). The Green functions used to form the self-energy $\Sigma(\mathbf{K}, \omega)$ are coarse grained, or

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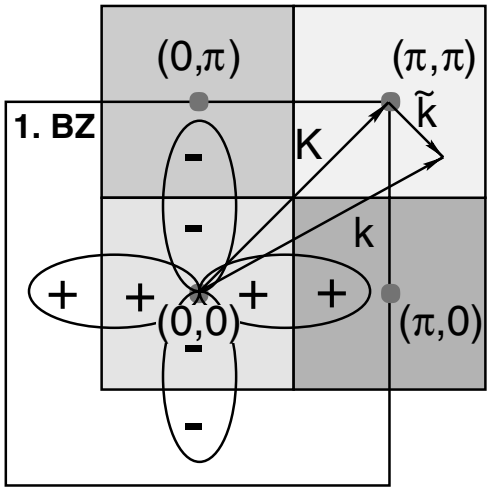

FIG. 1. Choice of the $N_c = 4$ cluster $\mathbf{K}$ points (filled circles), corresponding coarse graining cells (shown by different fill patterns), and a sketch of the d-wave symmetry of the order parameter.

averaged over the momenta $\mathbf{K} + \tilde{\mathbf{k}}$ surrounding the cluster momentum points $\mathbf{K}$ (cf. Fig. 1).

Thus, the *coarse grained* Green function is

$$\hat{\bar{G}}(\mathbf{K}, \omega) = \frac{N_c}{N} \sum_{\tilde{\mathbf{k}}} \hat{G}(\mathbf{K} + \tilde{\mathbf{k}}, \omega), \qquad (1)$$

where the sum runs over all vectors $\mathbf{k} = \mathbf{K} + \tilde{\mathbf{k}}$ within a cell around the cluster momentum $\mathbf{K}$. Note that the choice of the coarse grained Green function has two well-defined limits: For $N_c = 1$ the sum over $\tilde{\mathbf{k}}$ runs over the entire Brillouin zone, and $\hat{\bar{G}}$ is the local Green function, thus the DMFA algorithm is recovered. For $N_c = \infty$ the $\tilde{\mathbf{k}}$ summation vanishes and the DCA becomes equivalent to the exact solution. The dressed lattice Green function takes the form

$$\hat{G}(\mathbf{k}, \omega) = [\omega \tau_o - \bar{\epsilon}_{\mathbf{k}} \tau_3 - \hat{\Sigma}(\mathbf{K}, \omega)]^{-1}, \qquad (2)$$

with the self-energy $\hat{\Sigma}(\mathbf{k}, \omega)$ approximated by the cluster self-energy $\hat{\Sigma}(\mathbf{K}, \omega)$. To allow for a possible transition to the superconducting state we utilized the Nambu-Gorkov matrix representation [14] in (2) where the self-energy matrix $\hat{\Sigma}$ is most generally written as an expansion $\hat{\Sigma} = \sum_i \Sigma_i \tau_i$ in terms of the Pauli matrices τ_i. The diagonal components of $\hat{\Sigma}$ represent quasiparticle renormalizations, whereas the off-diagonal parts are nonzero in the superconducting state only.

Since the self-energy $\hat{\Sigma}(\mathbf{K}, \omega)$ does not depend on the integration variable $\tilde{\mathbf{k}}$, we can write

$$\hat{\bar{G}}(\mathbf{K}, \omega) = [\omega \tau_o - \bar{\epsilon}_{\mathbf{K}} \tau_3 - \hat{\Sigma}(\mathbf{K}, \omega) - \hat{\Gamma}(\mathbf{K}, \omega)]^{-1}, \qquad (3)$$

where $\bar{\epsilon}_{\mathbf{K}} = N_c/N \sum_{\tilde{\mathbf{k}}} \epsilon_{\mathbf{K}+\tilde{\mathbf{k}}}$. This has the form of the Green function of a cluster model with periodic boundary conditions coupled to a dynamic host described by $\hat{\Gamma}(\mathbf{K}, \omega)$. Here we employ the noncrossing approximation (NCA) [15] to calculate the cluster Green function and self-energy, respectively. A detailed discussion of the NCA algorithm applied to the cluster model for the paramagnetic state was given in [12]. Here it was shown that the NCA has only systematic errors of the order of $1/N_c^3$, while, e.g., QMC has systematic and statistical errors of the same order of magnitude. In addition, the NCA is especially well suited to address the dynamics of the strong coupling regime, where the application of QMC is limited by the sign problem. For the superconducting state the NCA has to be extended in order to account for the hybridization to the anomalous host, which couples cluster states with different particle numbers.

The self-consistent iteration is initialized by calculating the coarse grained average $\hat{\bar{G}}(\mathbf{K})$ [Eq. (1)] and with Eq. (3) the host function $\hat{\Gamma}(\mathbf{K})$, which is used as input for the NCA. The NCA result for the cluster self-energy $\hat{\Sigma}(\mathbf{K})$ is then used to calculate a new estimate for the coarse grained average $\hat{\bar{G}}(\mathbf{K})$ [Eq. (1)]. The procedure continues until the self-energy converges to the desired accuracy.

Results.—We investigate the single particle properties of the doped 2D Hubbard model,

$$H = \sum_{ij,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (4)$$

where $c_i^{\dagger}$ (c_i) creates (destroys) an electron at site i with spin σ and U is the on-site Coulomb repulsion. For the Fourier transform of the hopping integral t_{ij} we use

$$\epsilon_{\mathbf{k}} = \epsilon_o - \mu - 2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y, \qquad (5)$$

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 description of the high-T_c cuprates.

To allow for symmetry breaking we start the iteration procedure with finite off-diagonal 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 2×2 cluster ($N_c = 4$), the smallest cluster size incorporating nearest neighbor correlations. For the set of cluster points we choose $\mathbf{K}_{\alpha l} = l\pi$, where $l = 0, 1$ and $\alpha = x$ or y. Figure 1 illustrates this choice of $\mathbf{K}$ 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 (π, π), whereas the anomalous parts at the points $(0, \pi)$ and $(\pi, 0)$ should be finite with opposite signs.

Figure 2 shows a typical result for the local density of states (DOS) in the superconducting state along with the anomalous coarse grained Green function $\bar{G}_{12}(\mathbf{K}, \omega) = N_c/N \sum_{\tilde{\mathbf{k}}} \langle\langle c_{\mathbf{K}+\tilde{\mathbf{k}}\uparrow}; c_{-(\mathbf{K}+\tilde{\mathbf{k}})\downarrow} \rangle\rangle_{\omega}$ at the cluster $\mathbf{K}$ points for

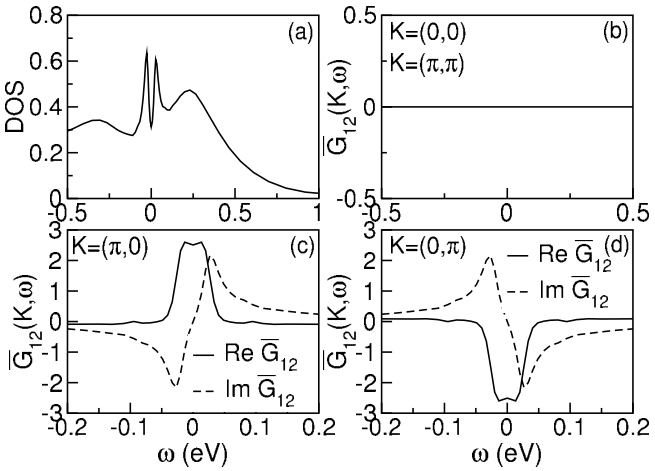

FIG. 2. (a) The local density of states (DOS) near the Fermi energy and the anomalous coarse grained Green functions at the cluster points (b) $\mathbf{K} = (0,0)$ and $\mathbf{K} = (\pi,\pi)$, (c) $\mathbf{K} = (\pi,0)$ and (d) $\mathbf{K} = (0,\pi)$ in the superconducting state. The nearest neighbor 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.

$t' = 0$, temperature $T = 137$ K, and doping $\delta = 0.19$. The anomalous coarse grained Green function vanishes at the cluster points $(0,0)$ and (π,π) 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 DOS depicted in Fig. 2a, where we show the lower subband of the full spectrum near the Fermi energy. It displays the superconducting state pseudogap at zero frequency as expected for a d-wave order parameter.

Figure 3 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 size of the superconducting state pseudogap, measured as the peak to peak distance, as well as the density of states at the Fermi energy does 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.

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 $\bar{G}_{12}(\mathbf{K},\tau = 0) = N_c/N \sum_{\tilde{\mathbf{k}}} \langle c_{\mathbf{K}+\tilde{\mathbf{k}}\uparrow} c_{-(\mathbf{K}+\tilde{\mathbf{k}})\downarrow} \rangle$ for $\mathbf{K} = (\pi,0)$. This number as a measure of the superconducting gap shows exactly the same behavior as the density of states.

The anomalous components $\bar{G}_{12}(\mathbf{K},\omega)$ become smaller with increasing temperature and eventually vanish at a

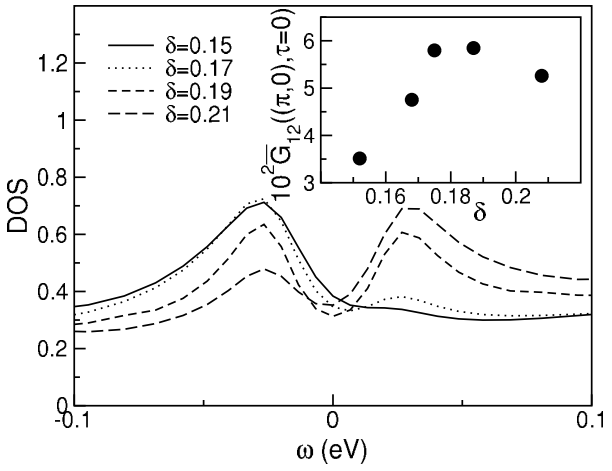

FIG. 3. Density of states in a narrow region at the Fermi energy for the same parameters as in Fig. 2 but for various dopings. The gap size and the density of states at $\omega = 0$ are independent of doping. Inset: Equal time coarse grained anomalous Green function $\bar{G}_{12}(\mathbf{K},\tau = 0)$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

critical temperature T_c depending on the set of parameters. The phase diagram is shown in Fig. 4. 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 δ. 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 breakdown of the NCA at very low temperatures we are not able to extend the phase diagram beyond the region shown in Fig. 4. This means, in particular, that we cannot predict reliable values for $\delta_c(T = 0)$, beyond which superconductivity vanishes.

Another question concerns magnetic phases, especially antiferromagnetism. There is indeed a region of antiferromagnetism around half filling for a 2×2 cluster with

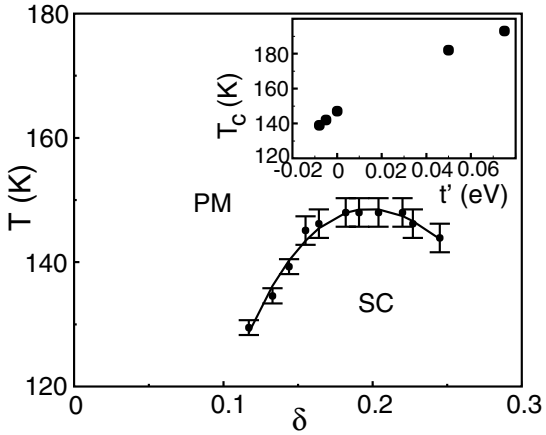

FIG. 4. Temperature-doping phase diagram for the 2D Hubbard model via DCA for a $N_c = 4$ cluster. The nearest neighbor hopping $t = 0.25$ eV, next nearest neighbor hopping $t' = 0$, and the Coulomb repulsion $U = 3$ eV. The error bars result from the finite resolution in temperature. Inset: Transition temperature $T_c(t')$ for fixed doping $\delta = 0.18$ as a function of the next nearest neighbor hopping amplitude t'.

Néel temperatures above T_c. However, T_N drops quickly with doping, and we do not find any long-range order other than superconductivity close to optimal doping. For a 2D system we do not expect to find antiferromagnetism at finite T, while superconductivity can prevail as a Kosterlitz-Thouless transition. Indeed, preliminary results for larger clusters show that T_N decreases with cluster size, in accordance with the theorem of Mermin and Wagner, while T_c weakly increases. For this reason we do not consider antiferromagnetism here. A finite hopping matrix element along the c axis, thus introducing three dimensionality, stabilizes T_N. Work along this line is in progress.

The inset of Fig. 4 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 $t' > 0$. At first this result seems counterintuitive as decreasing t' would tend to increase the density of states at the Fermi surface and so increase T_c, and a $t' < 0$ would seem to provide a mixing between next nearest neighbor sites that promotes d-wave symmetry. However a similar result was found by White *et al.* [16]. They argue that, due to the short-ranged antiferromagnetic correlations, the relative phase between the states with N and $N + 2$ holes already has d-wave symmetry, therefore $t' > 0$ provides a mixing compatible with d-wave pairing.

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 off-diagonal 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.

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