Enhancement of Superconducting Pairing by Inhomogeneity

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Inhomogeneous s-wave superconductivity is studied in the two-dimensional, square lattice attractive Hubbard Hamiltonian using the Bogoliubov-de Gennes (BdG) mean field approximation. We find that at weak coupling, and for densities mainly below half-filling, inhomogeneity of the interaction enhances the zero temperature pairing amplitude and that the superconducting T_c can also be significantly increased. These effects are observed for stripe, checkerboard, and even random patterns of the attractive centers, suggesting this is a general effect. Monte Carlo calculations which reintroduce some of the fluctuations neglected within the BdG approach see the same enhancement, both for the attractive Hubbard model and a Hamiltonian with d-wave pairing symmetry.

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One of the main themes of recent studies of strongly correlated electronic systems is the importance of spatial inhomogeneities. These can result either from intrinsic quenched disorder in the system, as in the metal-insulator transition in two dimensions[1, 2], or arise spontaneously in an otherwise translationally invariant system. For example, holes doped into the high temperature superconductors, (HTS) appear not to spread out uniformly in the CuO_2 planes, but instead arrange themselves in the form of stripes, checkerboard or perhaps even more exotic structures.[3] Besides the cuprate superconductors, such spatially varying density and spin structures are also key features in the physics of the manganites [4] and cobaltites.[5]

Considerable theoretical work on the interplay between spatial inhomogeneity, magnetism, and superconductivity has utilized the repulsive Hubbard and t-J Hamiltonians.[6–8] For the $2D$ square lattice these models are known to display antiferromagnetism at half-filling, and, although it is less certain, perhaps also d-wave superconductivity when doped. There is considerable evidence that they also might possess inhomogeneous stripe or checkerboard ground states,[7, 8] but it appears that such phases are rather close in energy to homogeneous ones, and dependent on details such as the choice of boundary conditions. While DMRG treatments[7] provide detailed information on the real space charge, spin, and pairing orders, the precise nature of the interplay, and whether the different orders compete or cooperate, remains unclear. The enhancement of the superconducting transition temperature T_c by local inhomogeneity has also been demonstrated by Martin *et al.*, in Ref.[9] where they find that the inhomogeneity which is incommensurate with the Fermi surface nesting vectors enhances T_c compared to its value for the uniform pattern.

In this paper we address the general issue of whether inhomogeneous regions of attraction favor superconductivity, either by increasing the zero temperature pairing amplitude or the transition temperature. In many of the systems for which this question is fundamental, such as the cuprate superconductors mentioned above, the situation is complicated by the presence of other types of order such as antiferromagnetism, exotic spin-gap phases, and nontrivial d-wave symmetry of the superconducting order parameter. Rather than using a model like the repulsive Hubbard Hamiltonian which incorporates this full richness, it is useful to study the problem first in a more simple context. Here we will present a solution of the inhomogeneous Bogoliubov-de Gennes (BdG) equations for the attractive Hubbard Hamiltonian,

$$H = -\ t \sum_{<ij>\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) - \ \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i,\sigma} - \sum_i |U_i| n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

with t the hopping amplitude, μ the chemical potential and U_i the local attractive interaction between the fermions of opposite spins residing on the same lattice site i. Our focus will be on inhomogeneous patterns in the interaction U_i. As has been discussed,[10] the interaction in the attractive Hubbard model can be thought of as a phenomenological one, originating, for example, from integrating out a local phonon mode.

The two-dimensional uniform attractive Hubbard model is known to yield degenerate superconductivity and charge density wave (CDW) long range order at half-filling and zero temperature.[11] However, away from half-filling, the CDW pairing symmetry is broken and superconductivity is more favorable. The transition is of the Kosterlitz-Thouless type with $T_c > 0$.

Within the BdG mean field decomposition, we replace the local pairing amplitude and local density by their average values,

$$\Delta_i = \langle c_{i\uparrow} c_{i\downarrow} \rangle \qquad \langle n_{i\sigma} \rangle = \langle c^\dagger_{i\sigma} c_{i\sigma} \rangle \, , \tag{2}$$

and arrive at the quadratic effective Hamiltonian

$$\mathcal{H}_{eff} = - \; t \sum_{<ij>,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i,\sigma}) - \sum_{i\sigma} \tilde{\mu}_i c^\dagger_{i\sigma} c_{i\sigma} - \sum_i |U_i| \big[\Delta_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \Delta^*_i c_{i\downarrow} c_{i\uparrow} \big] \, , \tag{3}$$

where $\tilde{\mu}_i = \mu + |U_i| \langle n_i \rangle /2$ includes a site-dependent Hartree shift with $\langle n_i \rangle = \sum_\sigma \langle n_{i\sigma} \rangle$. All energies are referenced to $t = 1$.

We compare the tendency for superconductivity when the system is homogeneous, namely, the same attraction $-U$ occurs on all lattice sites, with cases when sites with attraction are mixed with sites where the attraction is absent, i.e., $U_i = 0$. Specifically, we have studied systems in which $-U$ sites are randomly distributed on the lattice [12] or arranged in checkerboard and stripe patterns. In all these three inhomogeneous patterns, exactly half of the lattice sites carry interaction, and the interacting sites carry twice the value of U as in the case of the uniform pattern. This choice of inhomogeneity fraction facilitates comparison with checkerboard and stripe patterns, which similarly divide into two sublattices of equal size. However, the study of the case of more general fractions of random $U = 0$ sites is also interesting.

For the case of random patterns, we must repeatedly diagonalize a matrix of dimension twice the number of spatial sites, in order for the self consistency conditions of Eq. 2-3 to converge and then to average over different disorder realizations. This limits the system size to 10^2 to 10^3 sites. On the other hand, for the periodic checkerboard and stripe patterns, the Hamiltonian becomes block diagonal in momentum space and we can study lattices with millions of spatial sites. This is important at small U where it is known that finite size effects can be more significant, and where, as it turns out, the interesting enhancements of pairing are seen in our model.

This conventional mean-field approach does not capture the Kosterlitz-Thouless nature of the phase transition in two dimensions. Nevertheless, as was shown recently, this weakness can be repaired upon regarding the local pairing amplitudes as *complex* variables and performing a finite temperature Monte Carlo integration over the associated amplitude and phase degrees of freedom. [13] Unlike BCS, this approach, referred to as the Monte Carlo mean field (MCMF), also allows identification of the weak and strong coupling regimes via the phase correlation function. We will use this Monte Carlo technique as an independent confirmation of our results.

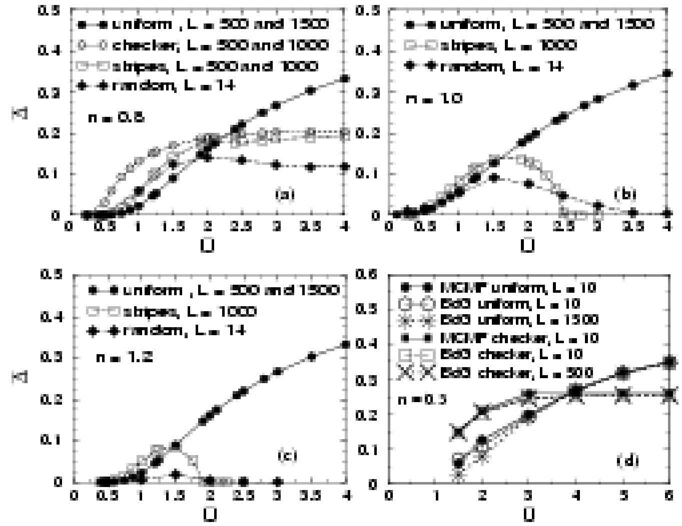

FIG. 1: Variation of the mean zero temperature pairing amplitude $\bar{\Delta}$, versus mean interaction $\bar{U}$, for (a) below half-filling ($n = 0.8$), (b) half-filling ($n = 1.0$), and (c) above half-filling ($n = 1.2$). There is a substantial enhancement of $\bar{\Delta}$ for weak couplings and all types of inhomogeneities at $n = 0.80$. There is no pairing at $n \geq 1$ in the checkerboard case. For the stripe, checkerboard, and uniform patterns, data are fully converged on the momentum space grid. That is, data for the indicated lattice sizes lie on top of each other. For the random pattern it is not possible to study large lattices, and a single size, $L = 14$ is shown. Panel (d) compares the MCMF results ($T \approx 0$) at $L = 10$ with their BdG counterparts at $L = 10$, 500 and 1500 for the uniform and checkerboard patterns.

In Fig. 1, the mean pairing amplitude is plotted versus mean interaction for different inhomogeneous patterns and several electron dopings at $T = 0$. For the doping of $n = 0.8$, as depicted in panel (a), the inhomogeneity *enhances* superconductivity in the region below the maximum value of $\bar{U}_{(r=1)} \approx 2.0$ with $r = \bar{\Delta}_{\rm inhomog}/\bar{\Delta}_{\rm uniform}$. At half-filling in panel (b), enhancement for the stripe pattern terminates at slightly smaller values of $\bar{U}_{(r=1)} \approx 1.5$ and at the same time, the magnitude of $\bar{\Delta}_{(r=1)}$ has also diminished. Moreover, there is an upper critical $\bar{U}_c$ above which superconductivity is obliterated by inhomogeneity. For the checkerboard pattern at half-filling in particular, $\bar{\Delta}$ becomes zero as one enters the insulating CDW phase of static pairs. The enhancement is even further suppressed for the doping of $n = 1.2$ above half-filling in panel (c) for random and stripe patterns and $\bar{\Delta}$ for the checkerboard pattern still remains infinitesimal over almost the entire range of $\bar{U}$. Panel (d), makes a comparison between the MCMF results, in which phase fluctuations have been introduced into the mean field calculations with their BdG counterparts. For the lattice size of $L = 10$, results show satisfying agreement between the two approaches. While the MCMF method remains limited to relatively small lattice sizes, BdG allows us to invoke lattice sizes as large as $L = 1500$ to reduce the

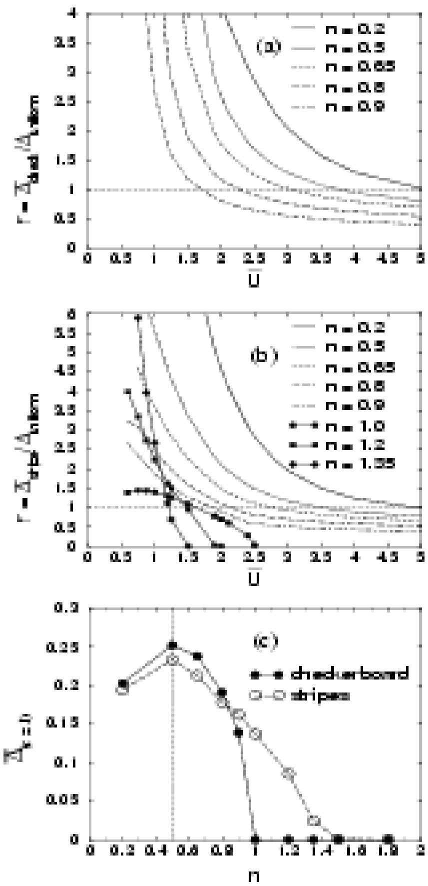

FIG. 2: Panel (a): the ratio $r = \bar{\Delta}_{\rm check}/\Delta_{\rm uniform}$ as a function of $\bar{U}$ and different dopings of electrons at $T = 0$. Panel (b): the same results as for panel (a) for the ratio $r = \bar{\Delta}_{\rm stripe}/\Delta_{\rm uniform}$. Panel (c): pairing amplitude (beyond which the enhancement ceases) versus the electron doping. The maximum value of coupling for which enhancement is observed shifts to higher values as n moves away from half-filling. A factor of three to four enhancement for the zero temperature pairing amplitude can occur due to inhomogeneity at weak coupling. Lattice sizes of $L = 1500$ for the uniform and $L = 500$ and 1000 for inhomogeneous patterns were utilized.

finite size effects at small $\bar{U}$ values. As observed in panel (d) of Fig. 1, the finite size effects are more significant for the uniform pattern when $\bar{U} \lesssim 3.0$ and less severe for the checkerboard. The good agreement between these two approaches helps justify both the application and results of the BdG technique.

Fig. 2 illustrates further the size of the enhancement due to inhomogeneity by showing the ratio of the inhomogeneous zero temperature pairing amplitude to its homogeneous value. Data over a broad range of densities are provided. For the checkerboard pattern in panel (a), as the doping changes from $n = 0.2$ to $n = 0.9$, the intersection point of the ratio $r = \bar{\Delta}_{\rm check}/\Delta_{\rm uniform}$ and unity line is shifted towards smaller $\bar{U}_{(r=1)}$. Precisely at half-filling, $\bar{\Delta}$ for the checkerboard pattern vanishes. For stripes, however, as shown in panel (b), the enhancement shift towards smaller $\bar{U}_{(r=1)}$ continues at half-filling and also above half-filling up to almost $n = 1.35$. Panel (c) shows the value of the pairing amplitude $\bar{\Delta}_{(r=1)}$ as a function of the electron doping. The enhancement for both the checkerboard and stripe patterns is maximum near $n = 0.5$, making it close to an optimal doping value for enhancement.

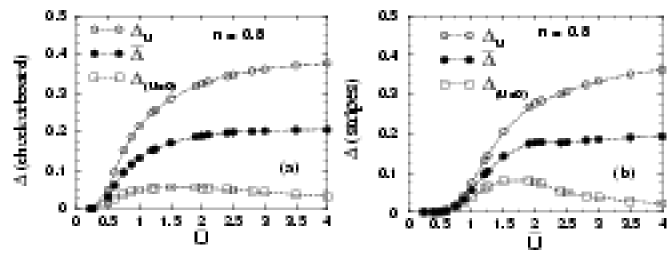

FIG. 3: Variation of the pairing amplitude versus the mean interaction $\bar{U}$ at $T = 0$. Panel (a) shows $\bar{\Delta}$ as the average of $\Delta_{\rm U}$ and $\Delta_{\rm (U=0)}$ for the checkerboard pattern at $n = 0.8$ and the same for stripes in panel (b). The enhancement of pairing by inhomogeneity is seen to arise from a proximity effect whereby significant pair amplitude is induced on the $U = 0$ sites by the $U \neq 0$ sites. The region of pairing enhancement disappears when the pairing amplitude on the $U = 0$ sites turns over and begins to decrease. Lattice sizes of $L = 500$ and 1000 were utilized.

The lack of superconductivity in the checkerboard pattern at half-filling is associated with the formation of a competing, insulating CDW phase. This can be seen directly in the density of states as a gap develops at the Fermi energy despite the fact that $\Delta_{sc} = 0$. The occupation of sites in real space becomes increasingly disparate as U increases, with the sites with $U \neq 0$ becoming fully packed with $n_U \approx 2.0$, while the non-interacting sites become empty, $n_{(U=0)} \approx 0.0$. For stripes at half-filling also, at large enough values of $\bar{U}$ superconductivity is obliterated. Above half-filling, however, when the order parameter vanishes for both the checkerboard and stripes, the density of states remains finite at the Fermi energy, indicating a metallic phase.

The proximity effect for the non-interacting sites neighbored by the interacting sites plays a major role in the enhancement due to inhomogeneity. In Fig. 1, panel (a), the enhancement of $\bar{\Delta}$ for the checkerboard and stripe patterns at $n = 0.8$ terminates near $\bar{U}_{(r=1)} \approx 2.0$. In panels (a) and (b) of Fig. 3, $\bar{\Delta}$ for both these two patterns has been plotted as the average of the pairing amplitudes on interacting and non-interacting sites. Due to the proximity effect, even in the absence of interaction on a lattice site, there exists a finite value of pairing amplitude through the tunneling effect from its neighboring interacting sites. As observed in panels (a) and (b) in Fig. 3, while $\Delta_{\rm U}$ for both the checkerboard and stripe patterns consistently increases as a function of $\bar{U}$,

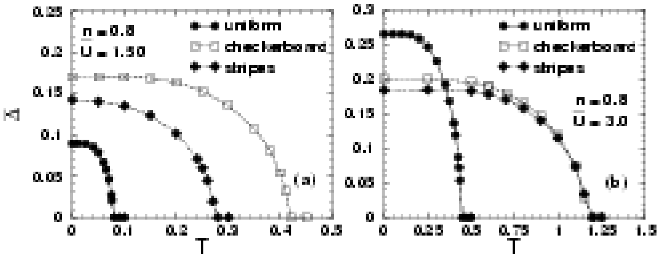

FIG. 4: Variation of the pairing amplitude versus temperature T for $n = 0.8$. Panel (a): $\bar{\Delta}$ as a function of T for $\bar{U} = 1.5$ where inhomogeneity enhances superconductivity for the checkerboard and stripe patterns at $T = 0$ (Fig. 1, panel (a)). Panel (b): the same results for $\bar{U} = 3.0$. Lattice sizes of $L = 1500$ for the uniform and $L = 500$ and 1000 for inhomogeneous patterns were utilized.

$\Delta_{(U=0)}$ increases up to $\bar{U}_{(r=1)} \approx 2.0$ where according to panel (a) in Fig. 1, the enhancement terminates. $\Delta_{(U=0)}$ then falls off for larger $\bar{U}$ values. Hence, while $\Delta_{(U=0)}$ increases with $\bar{U}$, there is enhancement in superconductivity for the average of Δ_U and $\Delta_{(U=0)}$, i.e., $\bar{\Delta}$.

Inhomogeneity also leads to the enhancement of the superconducting transition temperature T_c. According to Fig. 1, panel (a), at $\bar{U} = 1.5$, $\bar{\Delta}(T = 0)$ is enhanced due to inhomogeneity but at $\bar{U} = 3.0$, the uniform pattern wins over inhomogeneity by yielding a larger value of $\bar{\Delta}$. Fig. 4 illustrates the collapse of $\bar{\Delta}$ as the temperature is increased for the uniform, checkerboard and stripe patterns. In panel (a) of Fig. 4 corresponding to $\bar{U} = 1.5$, the enhancement due to inhomogeneity persists through all values of finite T up to T_c which is significantly larger for the inhomogeneous patterns. In panel (b) of Fig. 4 corresponding to $\bar{U} = 3.0$, at $T = 0$, $\bar{\Delta}$ for the uniform pattern is significantly larger than its inhomogeneous counterparts. However, because of the substantial enhancement of T_c due to inhomogeneity, for values of $0.5 \lesssim T \lesssim 1.25$, there exists an enhancement region for $\bar{\Delta}$ for inhomogeneous patterns. For the uniform pattern, we find the T_c in very good agreement with the BCS value, $k_b T_c \approx (\Delta(0)U)/1.76$, as expected for our mean field treatment. Note that the the enhancement of T_c by inhomogeneity would appear to be even more dramatic if we compared the inhomogeneous curves against their BCS counterparts with the same $\Delta(T = 0)$. A similar increase in T_c upon introducing a checkerboard pattern is found in the MCMF calculations as well due to the loss of long-range phase coherence. This is particularly significant because the MCMF incorporates the the subtle nature of the superconducting transition in $2D$ discussed earlier. We have also independently confirmed that our conclusions and arguments equally apply for a model with nearest-neighbor attraction, leading to a d-wave SC close to half-filling, which reflects the cuprates' phenomenology more truthfully.[13]

In summary, we have shown that for the attractive Hubbard model on a square lattice, inhomogeneity in the pattern of interacting sites results in the enhancement of the superconducting order parameter over a significant range of electron doping and interaction values. This enhancement has been verified specifically for the checkerboard, stripe and random patterns and in all likelihood is a general result. The enhancement is due to the proximity effect, i.e., the tunneling effect of the Cooper pairs from the interacting sites leading to finite order parameter values even on non-interacting sites.This conclusion is supported by the enhancement occurring at weak coupling, where the coherence length is large rather than in the strong coupling regime of preformed pairs. For the checkerboard and stripes, we find that the order parameter associated with $\bar{U}_{(r=1)}$ reaches its maximum near the doping value of $n = 0.5$, being close to the optimum value for n. The checkerboard pattern at half-filling shows insulating phase characteristics even at very small interactions and hence no superconductivity while for the stripes at half-filling, the superconductivity persists up to a certain $\bar{U}_c$ before it vanishes. Both the checkerboard and stripes at half-filling exhibit CDW long range order at large enough $\bar{U}$ values. Above half-filling, the checkerboard and stripe patterns are believed to be in a metallic phase when not superconducting. The agreement between the BdG results and the MCMF calculations justifies the application and conclusions of the BdG approach within the small $\bar{U}$ regime. Finally, inhomogeneity is also responsible for the significant enhancement in the phase transition temperature T_c. Counterintuitively, this enhancement in T_c occurs even for values of $\bar{U}$ for which the enhancement of the order parameter has already terminated at $T = 0$. However, in this weak coupling parameter regime, T_c is a supralinearly increasing function of U, so it may be that in the inhomogeneous system, the sites with larger U produce a nonlinear enhancement relative to Tc of the homogeneous system and, through the proximity effect, drag the $U_i = 0$ sites along with them.

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