Robustness of d-Density Wave Order to Nonmagnetic Impurities

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Effect of finite density of nonmagnetic impurities on a coexisting phase of d-density wave (DDW) order and d-wave superconducting (DSC) order is studied using Bogoliubov-de Gennes (BdG) method. The spatial variation of the inhomogeneous DDW order due to impurities has a strong correlation with that of density, which is very different from that of DSC order. The length scale associated with DDW is found to be of the order of a lattice spacing. The nontrivial inhomogeneities are shown to make DDW order much more robust to the impurities, while DSC order becomes very sensitive to them. The effect of disorder on the density of states is also discussed.

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\textbf{a. Introduction} One of the recent proposals in the context of high temperature cuprates is that a true broken symmetry state dubbed as d-density wave state (DDW) is responsible for the pseudogap phenomena.\textsuperscript{[1]} This phase was first suggested in relation to the excitonic insulators\textsuperscript{[2]}, and it was found as one of the ground states of the t-J type model.\textsuperscript{[3]} The DDW is a particle hole condensate with angular momentum 2. The ordered state can be characterized by the circulating current arranged in an alternating pattern on a square lattice. The inhomogeneous DDW order due to impurities has a strong spatial structures of the order parameter\textsuperscript{[11]}. Thus, the definite conclusion on the relevance of the DDW order to the cuprates requires more precise experiments on various doping concentrations of cuprates, and further theoretical studies on the properties of this new order. Especially, the effect of the nonmagnetic impurities on DDW order is an important subject to investigate, since any well-prepared cuprate sample contains an intrinsic disorder, minimally from non-stoichiometry.

The simplest possible description of the impurity effect is the self-consistent T-matrix approximation (SCTMA)\textsuperscript{[4]}. This mean field picture excludes not only the freedom of the ordered patterns, but also the interference of the impurities. Within this approximation, the thermodynamics were found to be identical to those of a d-wave BCS superconductor (DSC) in the unitary limit.\textsuperscript{[10]} From the density of states, one can see that electrons are localized close to the Fermi energy, and the change in the transition temperature is given by the Abrikosov-Gorkov formula known in BCS superconductors.\textsuperscript{[11]} Within the standard non-crossing approximation, the similarity between the DDW and DSC is based on the d-wave symmetry of the gap.

In this paper, we study the effect of impurities on DDW order and for the case where DDW coexists with DSC using Bogoliubov-de Gennes (BdG) technique. This method is the mean field approximation, but it allows spatial inhomogeneity in order parameter. In the case of the disordered DSC with a short coherence length, it was shown that the superfluid stiffness is significantly larger than that predicted by the SCTMA, due to the nontrivial spatial structures of the order parameter\textsuperscript{[11]}.

We found that the DDW order is more robust than the DSC order to the impurities, which cannot be understood within the conventional T-matrix approach. The physical ground for our findings will be discussed later.

\textbf{b. Model} We model two dimensional disordered DSC and DDW order by the following Hamiltonian.

\begin{equation}
\mathcal{H} = -t \sum_{<ij>,\alpha} (c_{i\alpha}^\dagger c_{j\alpha} + \text{h.c.}) + \sum_i (V(i) - \mu) n_i + J \sum_{<ij>} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j/4) + W \sum_{<ij>,\alpha,\beta} n_{i\alpha} n_{j\beta}. \tag{1}
\end{equation}

The first term is the kinetic energy which describes electrons, with spin \(\alpha\) at site \(i\) created by \(c_{i\alpha}^\dagger\), hopping between nearest-neighbors \(<ij>\) on a square lattice. The disorder potential \(V(i)\) in the second term is an independent random variable at each site which is either \(+V_0\), with a probability \(n_{\text{imp}}\) (impurity concentration), or zero, and \(\mu\) is the chemical potential. The last, interaction term \(J\) is chosen to lead to a coexisting DSC and DDW order ground state in the disorder-free system, where \(\mathbf{S}_i\) and \(n_i\) are the spin and density operators, respectively.

The mean field decomposition of the above Hamiltonian leads to following BdG equations\textsuperscript{[14, 15]}

\begin{equation}
\left(\begin{array}{c}
\xi \\
\Delta^* - \xi^*
\end{array}\right)
\left(\begin{array}{c}
u_n^* \\
u_n
\end{array}\right) = E_n \left(\begin{array}{c}
u_n^* \\
u_n
\end{array}\right), \tag{2}
\end{equation}

where \(\xi u_n(j) = -\sum_\delta \{t + \Psi(j;\delta)e^{-i\mathbf{Q}.\mathbf{r}_j}\} u_n(j + \delta) + (V(j) - \mu_j) u_n(j)\) and \(\Delta u_n(j) = \sum_\delta (\Delta(j + \delta;\delta) u_n(j + \delta)\), and similarly for \(v_n(j)\). The local DSC pairing \(\Delta\) and DDW \((\chi = \text{Im}\Psi)\) amplitudes on a bond \((j;\delta)\) are defined by

\begin{align}
\Delta(j;\delta) &= \frac{J + W}{4} (c_{j+\delta}^\dagger c_j + c_j^\dagger c_{j+\delta}^\dagger), \\
\Psi(j;\delta) &= \frac{J + 2W}{4} (c_{j+\delta}^\dagger c_j - c_j^\dagger c_{j+\delta}^\dagger) e^{-i\mathbf{Q}.\mathbf{r}_j}. \tag{3}
\end{align}

where \(\delta = \pm\mathbf{x}, \pm\mathbf{y}\). The inhomogeneous Hartee and Fock shifts are given by \(\mu_j = \mu + (\frac{J}{2} + W) \sum_\delta (n_{j+\delta})\) and \(\text{Re}(\Psi(j;\delta))\) respectively.
We numerically solve for the BdG eigenvalues $E_n \geq 0$ and eigenvectors $(u_n, v_n)$ on a lattice of $N$ sites with periodic boundary conditions. We then calculate the d-wave pairing amplitude $\Delta(j; \delta) = (J + W) \sum_n [u_n(j + \delta) v_n^*(j) + u_n(j) v_n^*(j + \delta)]/4$ and the DDW order and Fock shift as the imaginary and real parts of $\Psi(j; \delta) = (J + 2W) \sum_n [v_n^*(j) v_n(j + \delta) - u_n(j) u_n^*(j + \delta)]/4$ at $T = 0$, and the density $\langle n_j \rangle = 2 \sum_n |v_n(j)|^2$. These are fed back into the BdG equation, and the process iterated until self consistency is achieved for each of the (local) variables defined on the sites and bonds of the lattice. The chemical potential $\mu$ is chosen to obtain a given average density $\langle n \rangle = \sum_i \langle n_i \rangle / N$. We define the site dependent order parameters in terms of the bond variables as, $\Delta(j) = [\Delta(j; +\delta) - \Delta(j; +\bar{\delta}) + \Delta(j; -\delta) - \Delta(j; -\bar{\delta})]/4$ and similarly for $\chi(j)$.

We have studied the model at $T = 0$ for a range of parameters and lattice sizes up to $40 \times 40$. Here we focus on $J = 1.16$, and $W = 0.6$, in units of $t = 1$, with $\langle n \rangle = 0.95$ on systems of typical size $30 \times 30$. For these parameters, and $n_{\text{imp}} = 0$, the maximum DSC gap is $\Delta_{\text{max}} = 0.16$ and the maximum DDW gap is $\chi_{\text{max}} = 0.31$. In the pure system our calculations reproduce a phase diagram of $\Delta_{\text{max}}$ and $\chi_{\text{max}}$ as functions of filling similar to Ref. [13]. For the impurity potential we choose $V_0 = 100$, close to the unitary limit. The results are averaged over 10 different realizations of the random potential.

c. Effect of Impurity on DDW and DSC Orders We summarize our main results in Fig. (1), where we plot the disorder dependence of different orders (normalized to $n_{\text{imp}} = 0$ values). Let us first look at the line (a) that represents the behavior of $\chi$ as a function of $n_{\text{imp}}$ at half filling ($\langle n \rangle = 1$). At this filling DDW is the stable order and DSC order in fact vanishes for the pure system. Comparing the behavior of $\chi$ with the results from SCTMA calculations (represented by (c) curve) we see that the DDW order is more robust to impurities than predicted by SCTMA.

On the other hand, away from half filling when we force $\chi = 0$ in BdG equations, DSC becomes the surviving order and the $n_{\text{imp}}$ dependence of $\Delta$ is given by the (b) line, which in fact is very similar to $\chi$ in the (a) curve. Such robustness of the DSC order to impurity had been studied before [11], and it is attributed primarily to the fact that – each impurity affects superconductivity rather inhomogeneously by destroying SC order within a small region (of size determined by coherence length $\xi$) around it. Hence the long range order is not globally affected. We find from our current numerical results that similar picture holds for DDW order as well, and $\chi$ is also affected locally by impurity, keeping long range DDW order robust.

However, similar study for the coexisting phase of DSC + DDW order at $\langle n \rangle = 0.95$ reveals surprisingly that, superconducting order is severely affected by disorder (curve (e)) in the coexisting phase, much more so than in the absence of $\chi$. On the contrary, the DDW order (curve (d)) coexisting with DSC order becomes even more robust to impurities. In fact for low $n_{\text{imp}}$, $\chi$ even increases with impurity. The rest of the paper is organized towards the detailed understanding of these unexpected results.

From Fig. (1d) we saw that the DDW order increases for small $n_{\text{imp}}$. To get a further insight, we study the spatial structures of the order parameter (particularly at large $n_{\text{imp}}$) on the lattice for each impurity configuration. In Fig. (2a) we present a Grey-scale plot of $\chi$ on a typical $30 \times 30$ lattice at $n_{\text{imp}} = 0.06$ for a given realization of scatterers. The dark (light) regions represent larger (smaller) values of $\chi$. Comparing this structure with Fig. (2b), that gives the spatial distribution of $|\langle n \rangle - 1|$ for the same $n_{\text{imp}}$, we see that $\chi$ is large in space where local density is close to 1 (half filling). The strong spatial correlation between these two panels is striking, although it is not exact; the scale of modulation of $\chi$ is somewhat larger than that of density. However, the strong tie of local $\langle n \rangle$ and $\chi$ suggest that the length scale of fluctuation of $\chi$ would be governed by that of $\langle n \rangle$, which is rather small (of the order of $k_F^{-1}$). This can be understood as follows.

The length scale associated with the DDW order, $\xi_{\text{DDW}} \sim 1/\chi$. When impurity is introduced, the bond current attached to the impurity site is forced to be zero. So does the density. However, the bond current ”near” the impurity site is re-constructed to satisfy the current conservation, and one should note that the healing length is of order of a lattice spacing. How the magnitude of the re-constructed bond-current is determined? This magnitude is strongly related to the local density. The electron density depletes close to impurities and increases at locations far from it, to keep the average at the desired

FIG. 1: The evolution of $\Delta$ and $\chi$ (normalized by their pure values) with $n_{\text{imp}}$ is plotted under different conditions (see text).
value. Since at low disorder, a large number of sites attain \( \langle n_i \rangle \sim 1 \), \( \chi \) increases at those sites; the DDW order is most stable near half filling, where perfect nesting occurs for our model. As a result average \( \chi \) increases. At very large \( n_{\text{imp}} \), local density would be either much larger or smaller than 1, and \( \chi \) would decrease everywhere. This argument can be substantiated by looking into our results for each configuration of impurities.

For \( \langle n \rangle = 1 \), introduction of impurity makes local density only to deviate from half filling. As a result \( \chi \) decreases monotonically as found in Fig. (1a). The above argument for the behavior of DDW order with impurity is independent of the coexisting DSC order and we also found similar trend in \( \chi \) as in Fig. (1d) for \( \langle n \rangle < 1 \) even in the absence of DSC order, which is consistent with our picture. This shows that DDW order responds to the density fluctuations due to impurities. On the contrary, the DSC order in the presence of impurities is not related to the local density fluctuations as DDW is, even though the length scale, \( \xi_{\text{DSC}} \sim 1/\Delta \), which is of the order of a few lattice spacing for high temperature superconductors under considerations. The behavior of \( \Delta \) in the presence of impurities is shown to be related to the electron-hole mixing in the real space [13]: \( \Delta \) is large when the density is close to the chemical potential.

Fig. (2c) and (2d) presents the spatial structure of \( \Delta \) on lattice with the same \( n_{\text{imp}} \) configuration in the presence and absence of DDW order. We clearly see that the DSC is strongly suppressed by the impurities when coexisting with DDW order (as also observed in Fig. (1b) and (1e)). The existence of DDW strongly affect the strength of the DSC, because away from the impurities there are regions where the density is near half-filling, hence the DDW becomes strong. Strong DDW allows significant weight of \((\pi,\pi)\) scattering that mixes the + and − lobes of the DSC order and thereby DSC becomes weak. The regions of small density does not contribute to DSC order as well, due to the absence of enough electrons for pairing! Thus in the inhomogeneous coexistence phase DSC order is suppressed everywhere.

d. Averaged Density of States  Let us now study the (impurity) averaged density of states (DOS) \( N(\omega) \) for different \( n_{\text{imp}} \) for the case of only DDW order (Panel a) and coexisting DDW + DSC order (Panel b). For the pure system with only DDW order, \( N(\omega) \) is the standard d-wave DOS. With increasing \( n_{\text{imp}} \) we see that the gap-edge singularities get rounded off and a small accumulation of states is produced at the particle side of spectrum close to \( \omega = 0 \). The accumulation of electrons around a single impurity effectively provide impurity screening, which will produce enhanced states at the particle side of the spectrum. [13] Such resonances from each impurity con-
tribute to the average $N(\omega)$ and produce a broad band which is reflected as a bump in Fig. (3a). However, the strength of the DDW order is not affected much (given by the relative location of the two coherence peaks). At this point, we should emphasize that the DOS structure for impure DSC state is very different, where coherence peaks get strongly suppressed and a thin gap persists at $\omega = 0$ [11, 12], so that $N(0) = 0$ for all $n_{imp}$. From our results with DDW order, we find that $N(0) \propto n_{imp}$, which is in disagreement with the prediction of T-Matrix result ($N(0) \propto \sqrt{n_{imp}}$) [10].

In Fig. (3b), for coexisting DSC + DDW, a double-gap DOS is expected at $n_{imp} = 0$ [21]; superconducting gap at $\omega = 0$ and d-density wave gap at $\omega = \mu$. With increasing $n_{imp}$, DSC gap gets washed out and by $n_{imp} = 0.03$, $N(\omega)$ looks very similar for Fig. (3a) and (3b) (The overall shift for the later case is due to the particle-hole asymmetry). This demonstrates in a different way our main result, that the DSC order is very sensitive to impurity whereas DDW order is robust in the coexisting phase.

c. Summary and Discussion We studied the effect of nonmagnetic impurity on DDW ordered state using BdG technique. While the standard SCTMA indicates that the effect of impurity on DDW is similar to that on DSC, we found that the spatial variation of the DDW order has a strong correlation with that of density [Fig. (2a) and (2b)], and it is very different from that of DSC order [Fig. (2a) and (2c)]. We discussed that this occurs because the length scale associated with the DDW order is of order of a lattice spacing ($\sim 1/k_F$), which suggests that the spatial variation of DDW order is related to the density fluctuation, while the DSC order is related to particle-hole mixing. Therefore, the effect of impurity on the DDW order is very different from that of DSC order, which cannot be obtained from the standard SCTMA method.

When DSC and DDW coexist, it turns out that DDW order do not care about the existence of DSC and it still follows the density profile in the presence of impurity. However, DSC order would vanish almost everywhere [See Fig. (2c)] This is because in the region of larger density it is killed by DDW, and in the region of smaller density it is destroyed by disorder. Thus in the inhomogeneous media both DDW and impurity are acting to suppress the DSC order.

Our current picture brings out the unexpected results and their understanding at the mean field level; if the DDW phase exists in cuprates, the Bragg signal would be detected in neutron scattering measurements even in the presence of strong nonmagnetic impurity, while the width of the Bragg peaks depends on strength of impurity. However, the definite answer for its relevance to the cuprates requires the understanding of the role of strong correlation, and interplay between different competing orders, which warrants further studies.

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