Quasiparticle States around a Nonmagnetic Impurity in D-Density-Wave State of High-\(T_c\) Cuprates

Jian-Xin Zhu,\(^1\) Wonkee Kim,\(^2\) C.S. Ting,\(^1\) and J. P. Carbotte\(^2\)

\(^1\)Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204
\(^2\)Department of Physics & Astronomy, McMaster University, Hamilton, Ontario, Canada, L8S 4M1

Recently Chakravarty et al. proposed an ordered \(d\)-density wave (DDW) state as an explanation of the pseudogap phase in underdoped high-\(T_c\) cuprates. We study the competition between the DDW and superconducting ordering based on an effective mean-field Hamiltonian. We are mainly concerned with the effect of the DDW ordering on the electronic state around a single nonmagnetic impurity. We find that a single subgap resonance peak appears in the local density of state around the impurity. In the unitary limit, the position of this resonance peak is always located at \(E_r = -\mu\) with respect to the Fermi energy. This result is dramatically different from the case of the pure superconducting state for which the impurity resonant energy is approximately pinned at the Fermi level. This can be used to probe the existence of the DDW ordering in cuprates.

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Recently a \(d\)-density wave (DDW) state was proposed to model the pseudogap in the underdoped high-\(T_c\) cuprates\(^{12}\). The key feature of the DDW state is staggered orbital magnetic moments (i.e., staggered currents) which break parity and time-reversal symmetry as well as the translation invariance by one lattice constant and rotation by \(\pi/2\). This proposal of a new order parameter differs fundamentally from other theoretical ideas\(^{3–5}\) which break parity and time-reversal symmetry as well as the translation invariance by one lattice constant and rotation by \(\pi/2\). For which the staggered current is a fluctuating rather than a static quantity. Whether such a DDW state really exists in the phase diagram of high-\(T_c\) cuprates is an interesting theoretical question\(^{1}\). More recently, the SU(2)\(^{7}\) or U(1)\(^{8}\) mean-field theory of the \(t\)-\(J\) model predicted that the DDW order could exist in a vortex core.

An interesting question is the effect of a single nonmagnetic impurity on the DDW state. The single impurity problem in the superconducting state has been intensively studied both theoretically\(^{12}\) and experimentally\(^{13,14}\). However, the same problem has not been well studied in the pseudogap (PG) state, which has been indicated by STM\(^{16}\) and by ARPES experiments\(^{17}\). Currently, the origin of the PG state remains unclear. Experimentally it was also argued\(^{15}\) that in the underdoped cuprates the superconducting and pseudo gap coexist unlike in the pre-formed pair model\(^{19}\). The electronic states around a single impurity may serve as a local probe to distinguish between these scenarios. Within the \(T\)-matrix approximation, it was argued\(^{20}\) that, as long as the band density of states is depleted at the Fermi energy, the existence of impurity resonant states is robust regardless of the microscopic origin of the PG state. Note that, without invoking any particular model, the band density of states was assumed in Ref.\(^{20}\) to be symmetric with respect to the Fermi energy. This choice corresponds to the chemical potential \(\mu\) being zero in a two-dimensional tight-binding model with nearest-neighbor hopping. In addition, because of the lack of a specific model, the calculation of the local density of states (LDOS) around an impurity goes beyond the scope of that work. The purpose of this paper is to address this question within the DDW state, for which the LDOS around the impurity is calculated. Our main result is that, in the strong scattering limit, the position of the induced resonant state has a one-to-one correspondence to the chemical potential, which is dramatically different from the case of the superconducting state (and also of the pre-formed pair scenario), where the resonant energy is almost pinned at the Fermi energy. This prediction can be readily used by the STM experiments to detect for the DDW state in the underdoped cuprates.

We start with a phenomenological model including the intersite charge density wave order in a \(d\)-wave superconductor. One could also envision intersite spin density wave instead of the charge density order; however, as long as the density order is to be interpreted as a pseudogap the charge density order is more reasonable experimentally\(^{9}\). The effective Hamiltonian is written as:

\[
H = \sum_{ij} [-t + (-1)^i \frac{V_{ij}}{2} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} (U_i - \mu)c^\dagger_{i\sigma} c_{i\sigma} + \sum_{ij} \Delta_{ij} c^\dagger_{i\uparrow} c_{j\downarrow} + \Delta^*_{ij} c^\dagger_{j\downarrow} c_{i\uparrow}]. \tag{1}
\]

Here \(c^\dagger_{i\sigma}\) creates an electron with spin \(\sigma\) at site \(i\). The summation is over the nearest neighbors sites. \(t\) is the hopping integral and \(\mu\) is the chemical potential. \(U_i\) is introduced to model the potential scattering, if any, from impurities or defects. \(W_{ij}\) and \(\Delta_{ij}\) are, respectively, the DDW and DSC order parameters, which are determined by the self-consistent conditions:

\[
W_{ij} = \frac{(-1)^i V_{DDW}}{2} (c^\dagger_{i\sigma} c_{j\sigma} - c^\dagger_{j\sigma} c_{i\sigma}) , \tag{2}
\]

and
\[ \Delta_{ij} = \frac{V_{DSC}}{2} (c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow}), \]

where \( V_{DDW} \) and \( V_{DSC} \) are the interaction for the DDW and DSC channels. \((-1)^j\) in the ansatz Eq. (2) ensures that nesting takes place at half filling, and that \( W_{ij} \) is pure-imaginary. A. Ghosal et al. [2] have considered a Fock shift, which is similar with \( W_{ij} \) but does not have the site-dependent factor \((-1)^j\). A possible model for the Hamiltonian [3] is the \( t-J \) model. Applying the mean-field approximation and the ansatz for the density wave to the exchange interaction, one can obtain density and superconducting order. Introduction of an intersite interaction in addition to the exchange interaction gives different values of \( V_{DSC} \) and \( V_{DDW} \).

The mean-field Hamiltonian (3) can be diagonalized by solving the resulting Bogoliubov-de Gennes equations self-consistently

\[ \sum_j \left( \hat{H}_{ij} - \Delta_{ij} \right) \begin{pmatrix} u_n^{i*} \\ v_n^{i*} \end{pmatrix} = E_n \begin{pmatrix} u_n^i \\ v_n^i \end{pmatrix}, \]

where the single particle Hamiltonian \( \hat{H}_{ij} = -i \delta_{i+j} + (-1)^j W_{ij} + (U_i - \mu) \delta_{ij} \), and the self-consistency now reads

\[ W_{ij} = (-1)^j \frac{V_{DDW}}{2} \sum_n \text{Im} [u_n^i v_n^{i*} + v_n^i u_n^{i*}] \tanh \left( \frac{E_n}{2k_B T} \right), \]

and

\[ \Delta_{ij} = \frac{V_{DSC}}{2} \sum_n (u_n^i v_n^{i*} + v_n^i u_n^{i*}) \tanh \left( \frac{E_n}{2k_B T} \right). \]

**Competition between DDW and DSC orderings.** The phase diagram with the DDW and DSC orderings in Ref. [3] was constructed from experiments. Therefore, it is important to self-consistently study the phase diagram of a clean system with DDW and DSC channel interactions. Although the DDW state breaks the translation invariance by one lattice constant \( a \), it is invariant under the translation with spacing \( \sqrt{2}a \) along the diagonal directions of the square lattice. Hereafter we will measure the length in units of \( a \) and the energy in unit of \( t \). The site-dependent factor \((-1)^j\) enables us to consider the square lattice as a bipartite lattice. Choosing the basis cell with the size \( \sqrt{2} \times \sqrt{2} \), we solve the BdG equation (3) and find the eigenvalues \( E_k = \pm E_{1,2}(k) \) with \( E_{1,2}(k) = |(\xi_k + \mu)|^2 + \Delta_k^2 |^1/2, \)

where \( \xi_k = -2(\cos k_x + \cos k_y), \theta_k = 2W_{D}(\cos k_x - \cos k_y), \xi_k = \sqrt{\theta_k^2 + |W_k|^2}, \) and \( \Delta_k = 2\Delta_{D}(\cos k_x - \cos k_y). \) The eigenfunctions corresponding to \( E_{1,2}(k) \) are,

\[ \begin{pmatrix} u_k^\alpha \\ v_k^\alpha \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} (1 \pm \frac{W_{D,k}}{\sqrt{\theta_k |W_k|^2}}) \xi_k \\ \frac{1}{\sqrt{2}} (1 \mp \frac{\theta_k}{W_k}) \xi_k \end{pmatrix}, \]

Here \( u_k^\alpha = \frac{1}{\sqrt{2}} (1 \pm \frac{W_{D,k}}{\sqrt{\theta_k |W_k|^2}}) \xi_k \) and \( v_k^\alpha = \frac{1}{\sqrt{2}} (1 \mp \frac{\theta_k}{W_k}) \xi_k \), and \( \phi_{DDW} = \tan^{-1}(-iW_{D,k}/\xi_k) \) and \( \phi_{DSC} \) are the phase associated with the DDW and DSC orders. Substitution of these eigenfunctions into the self-consistent equations for DDW and DSC order parameter leads to:

\[ W_d = \frac{V_{DDW}}{4N_L} \sum_{k,\alpha} W_{d}(\cos k_x - \cos k_y) |\xi_k + (-1)^\alpha \mu| E_{\alpha} \tanh \left( \frac{E_{\alpha}}{2k_B T} \right), \]

\[ \Delta_d = \frac{V_{DSC}}{4N_L} \sum_{k,\alpha} \Delta_{d}(\cos k_x - \cos k_y) E_{\alpha} \tanh \left( \frac{E_{\alpha}}{2k_B T} \right), \]

where \( \alpha = 1, 2 \) and \( N_L \) is the number of the basis cells. Notice that at the fixed doping, the chemical potential itself is determined from \( \delta = 1 - n \) where the filling factor \( n = \frac{N}{N_L} \sum_{k,s} \{ f(E_\alpha) u_k^\alpha + \} \{ f(E_\alpha) v_k^\alpha \}. \) The solutions to the above equations have shown that the critical temperature \( T^0_{DDW} \) for the “bare” transition to the DDW state decreased more quickly than \( T^0_{DSC} \) for the DSC state. Therefore, only when the DDW channel interaction is larger than the DSC one, can there exist separated regions where either the DDW or DSC state is dominant. As a model calculation, we display in Fig. 3 the temperature versus doping phase diagram for \( V_{DDW} = 1.6 \) and \( V_{DSC} = 1.4 \). In the region of doping close to zero, the DDW state is dominant while in the region of \( \delta \) away from zero, the DSC state is dominant. In addition, we have a finite area of coexisting DDW+DSC phase. The size of the pure DDW region could be increased with a different choice of \( V_{DDW} \) and \( V_{DSC} \) but this is not expected to lead to important quantitative change. Also half filling in our model is not an insulating anti-ferromagnetic phase because we have not included any of this physics in our model so that the pseudogap state extends down to \( \delta = 0 \).

This competition can be understood from a phenomenological Ginzburg-Landau (GL) theory. The GL free energy density, in terms of both the DDW and DSC order parameters, can be constructed from a symmetry analysis:

\[ f = \alpha_{DSC} |\Delta_d|^2 + \alpha_{DDW} |W_d|^2 + \beta_1 |\Delta_d|^4 + \beta_2 |W_d|^2 + \beta_3 |\Delta_d|^2 |W_d|^2 + \beta_4 (\Delta_d^2 W_d^2 + \Delta_d^2 W_d^2) \],

where we assume \( \alpha_{DSC} = \alpha_{DSC}' (T - T^0_{DSC}) \) and \( \alpha_{DDW} = \alpha_{DDW}' (T - T^0_{DDW}) \), and \( \beta's \) are all positive. As an example, in the region where \( T^0_{DDW} > T^0_{DSC} \), the second phase transition temperature for the DSC ordering is renormalized by the pre-existing DDW order parameter:

\[ T_{DSC} = T^0_{DSC} - \frac{(\beta_3 - 3\beta_4)(T^0_{DDW} - T^0_{DSC})}{2\beta_2 \alpha_{DSC}' \alpha_{DSC}' - (\beta_3 - 3\beta_4)}. \]

Therefore, even if the “bare” critical temperatures for both ordering are very close to each other, the second-phase transition temperature for the appearance of DSC
(or DDW) order parameter can be strongly suppressed by the dominant DDW (or DSC) order parameter. At the mean-field level, we conclude that when $V_{DDW} > V_{DSC}$, the phase diagram is consistent with that proposed in Ref. [1]. Here we also would like to point out that the U(1) mean-field theory of the $t$-$J$ model gives rise to $V_{DDW} = 0.5J$ while $V_{DSC} = J$, which may explain the absence of the bulk DDW state in that model [1].

The LDOS around a single nonmagnetic impurity. The LDOS is given by:

$$\rho_t(E) = -2 \sum_n [\left| u_n^i \right|^2 f'(E_n - E) + \left| u_n^o \right|^2 f'(E_n + E)],$$

(11)

where a factor 2 arises from the summation over spin, and $f'(E) \equiv d f(E)/dE$ with the Fermi distribution function $f(E) = 1/(e^{E/k_B T} + 1)$. The LDOS $\rho_t(E)$ is proportional to the local differential tunneling conductance which can be measured by STM experiments [22]. In our numerical calculation, we take the supercell size $N_x = N_y = 32$ and the number of supercells $M = 6 \times 6$. Since we are most interested in identifying the qualitative difference in the electronic states around the impurity for the DDW and DSC states, the thermally broadening effect will not be considered here and the temperature is fixed at $T = 0.01$. For simplicity, we also use uniform order parameter as an input to diagonalize Eq. (9) and the suppression of the order parameter near the impurity is ignored. This approximation should be acceptable to answer the questions we ask here.

We first consider the case of weak or moderately strong impurity scattering. Figure 4 gives a plot of the LDOS spectrum directly on the single-site impurity (a) and on a site one lattice constant away (b) for a pure DDW state. When the impurity scattering is weak ($U_{0} = 4$), the LDOS on both the impurity site and on its nearest neighbor has a single peak below the Fermi energy. Although the LDOS at the impurity site is similar to the case of a weak nonmagnetic impurity in a pure DSC state [10,23], the LDOS displays a single resonant peak at the nearest neighbor site while the DSC shows a double-peak structure with one peak above and the other below the Fermi energy. When the impurity scattering becomes stronger ($U_{0} = 100$), the subgap resonant peak in the LDOS at the impurity site is shifted toward $E_c = 0$ with respect to the Fermi energy at the same time its amplitude at the impurity site is strongly suppressed because of the strong impurity scattering while at the nearest neighbor site it is strongly enhanced.

In the unitary limit, the energy position $E_c$ for the impurity resonant state in a pure DDW state is very sensitive to the chemical potential. In Fig. 3 the LDOS spectrum is plotted at the nearest-neighbor site for various values of $\mu$. We see in Fig. 3 that the resonant energy position is exactly equal to $E_r = |\mu|$ ($\mu < 0$), which is in sharply contrast to the case of a single impurity in a pure DSC state, where the resonant energy is not sensitive to the chemical potential and roughly zero (i.e., very close to the Fermi surface). This difference can be understood as follows: The energy dispersion for the pure DDW state $E_{1,2}(k) = \sqrt{\epsilon_k^2 + |W_k|^2} + \mu$ shows that the overall quasiparticle band is shifted by $\mu$ because of nature of the DDW state. Correspondingly, the resonant peak which always exists at the band center is shifted by $\mu$. However, due to the pairing mechanism, the quasiparticle for the pure DSC state, as given by $E_{1,2}(k) = [(\epsilon_k + \mu)^2 + \Delta_0^2]^{1/2}$, are always excited w.r.t. the Fermi surface instead of the band center. Consequently, the impurity induced resonant state has the energy almost pinned around the Fermi surface. Moreover, as in the case of a DSC state, we have found that the impurity resonant peak intensity of the LDOS in a pure DDW state exhibits the Friedel-like spatial oscillation: It has local maxima on the sublattice containing the nearest neighbors and local minima on the sublattice containing the impurity site itself.

Finally, in Fig. 4, the LDOS spectra at the nearest-neighbor site of a moderately strong impurity is plotted in a mixed state of DDW and DSC ordering. For a comparison, the LDOS spectrum at the same site is also displayed in a pure DSC state. In the pure DSC state, we have the double-peak structure with the intensity of the peak above the Fermi energy stronger than that below the Fermi energy. However, in the mixed state with both orderings present, the intensity of the peak below the Fermi energy is stronger than that above because the impurity scattering in the DDW order shifts the resonant peak below the Fermi energy.

In conclusion, we have studied the competition between the DDW and DSC ordering. The implication of the DDW state for the impurity resonant state has been discussed in detail. The qualitative difference found in the resonant state in the DDW ordering compared with that in the DSC state can be used as a smoking gun for the existence of the DDW state in high-$T_c$ cuprates. Experimentally, the existence of this state can be identified by (i) detecting whether the local differential tunneling conductance near a single weak or moderately strong nonmagnetic impurity exhibits a single rather than double subgap structure around the Fermi surface and (ii) detecting the position of the subgap resonant peak in the conductance near a unitary nonmagnetic impurity which will have a strong doping dependence. An STM measurement is most suitable for this test.

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FIG. 1. The temperature versus doping(δ) phase diagram obtained from the Hamiltonian with channel interaction $V_{DDW} = 1.6$ and $V_{DSC} = 1.4$.

FIG. 2. The LDOS spectrum at the impurity site (a) and at its nearest neighbor (b) in a pure DDW state for various strengths of the impurity scattering $U_0 = 4$ (red-solid line) and $U_0 = 100$ (green-dashed line). Also shown is the spectrum in a pure DSC state with $\Delta_d = 0.1$ (green-dashed line).

FIG. 3. The LDOS spectrum at the nearest neighbor of a unitary impurity in a pure DDW state for various values of the chemical potential $\mu = 0$ (red-solid line), $-0.1$ (green-dashed line), and $-0.2$ (blue-dash-dotted line). The other parameter values: $W_d = 0.1$, $U_0 = 100$, and $T = 0.01$.

FIG. 4. The LDOS spectrum at the nearest neighbor of a weak impurity in a mixed state of DDW and DSC orderings (red-solid line). The other parameter values: $W_d = 0.08$, $\Delta_d = 0.1$, $U_0 = 4$, $\mu = 0$, and $T = 0.01$. Also shown is the spectrum in a pure DSC state with $\Delta_d = 0.1$ (green-dashed line).
FIG. 2 Zhu et al.
Figure 3: Zhu et al.
\[ \rho_i(E) \]