

## Model of Quasiparticles Coupled to a Frequency-Dependent Charge-Density-Wave Order Parameter in Cuprate Superconductors

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We investigate a model where superconducting electrons are coupled to a frequency dependent charge-density wave order parameter  $\Delta_r(\omega)$ . Our approach can reconcile the simultaneous existence of low-energy Bogoljubov quasiparticles and high energy electronic order as observed in scanning tunneling microscopy (STM) experiments. The theory accounts for the contrast reversal in the STM spectra between positive and negative bias observed above the pairing gap. An intrinsic relation between scattering rate and inhomogeneities follows naturally.

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The phenomenon of charge ordering and its relation to superconductivity remains a puzzling issue in the physics of high- $T_c$  cuprates. Whereas the occurrence of charge inhomogeneities was early on evidenced by local probes and discussed in the context of electronic phase separation [1] Tranquada and co-workers [2] succeeded in probing a one-dimensional static spin and lattice modulation in a rare earth codoped lanthanum cuprate compound (LCO) by elastic neutron scattering. The unambiguous existence of an associated charge modulation has been established only more recently with resonant soft-x-ray scattering [3]. In other cuprate compounds the existence of charge ordering so far comes from surface sensitive probes, like scanning tunneling microscopy (STM) and angle-resolved photoemission spectroscopy (ARPES). STM experiments performed on bismuthate and oxchloride superconductors see a complex modulation of the local density of states (LDOS) both in the superconducting (SC) state [4–9] and above  $T_c$  [9–11]. In both cases one observes peaks in the Fourier transform of the real space LDOS at wave vectors  $Q = 2\pi/(4a_0) \dots 2\pi/(5a_0)$ , suggestive of checkerboard or stripe charge order. However, the debate is about the question whether these peaks are nondispersive in energy (and thus signature of “real” charge order) or follow a bias-dependent dispersion due to quasiparticle interference (QPI). In the latter case the spatial LDOS variations can be understood from the so-called octet model [4,12] which attributes the modulations to the elastic scattering between the high density regions of the Bogoljubov “bananas” in the superconducting state. Recent STM investigations [13,14] may resolve this apparent conflict since they suggest that both, dispersive and nondispersive scattering originates from different regions in momentum and energy space. The states in the nodal region which are well defined in  $k$  space and undergo a transition to a  $d$ -wave SC state below  $T_c$  are then responsible for the low-energy QPI structure of the LDOS, whereas the ill-defined  $k$ -space

“quasiparticle” states in the antinodal regions are responsible for the nondispersive charge order above some energy scale  $\Omega_0$ . It is therefore a key issue to understand the nature of this charge ordering, which seems particularly elusive, at least at low energies, both in STM and ARPES experiments.

In this Letter we propose a phenomenological model which captures the above physical scenario by considering a frequency dependent charge-density wave order parameter analogous to the frequency dependent superconducting order parameter of Eliashberg theory. By construction the order parameter vanishes on the Fermi surface so that for small energies the system appears homogeneous and the concept of QPI applies while for large energies it appears to be charge ordered. As a bonus, the system shows a strong high energy contrast reversal of the LDOS as a function of energy in agreement with experiments [15] and an intimate relation between inhomogeneities and quasiparticle scattering rate.

We consider here a two-dimensional system of SC itinerant electrons scattering with a charge-density-wave order parameter with an internal dynamics. This is phenomenologically represented by a retarded local self-energy where the space and frequency dependencies are factorized

$$\Sigma_{\mathbf{r}}^{\text{CDW}}(\omega) = \Delta_{\mathbf{r}}(\omega) \equiv \Delta_{\mathbf{r}}^0 + v_{\mathbf{r}}^2 f(\omega). \quad (1)$$

A conventional CDW without internal dynamics has  $f(\omega) = 0$  and  $\Delta_{\mathbf{r}}^0 \neq 0$ . The function  $f(\omega)$  describes the internal dynamics of the CDW, that is particle-hole correlations building the charge density wave are time dependent. The spatial dependence is implemented via the modulation of  $v_{\mathbf{r}}^2$ . We will restrict to  $\text{Im}f(\omega) > 0$ , and  $v_{\mathbf{r}}$  real, which ensures  $\text{Im}\Sigma_{\mathbf{r}}^{\text{CDW}} > 0$  as required for stability.

The internal dynamics can be motivated on the basis of a frequency dependent interaction, presumably of electronic origin and the same that originates superconductivity but which we do not need to specify. It implies that charge

piling is *retarded*, which is physically appealing since it reduces the Coulomb penalty as in the Eliashberg theory of superconductivity. Such retardation effects are especially important for cuprates which are characterized by a large Coulomb repulsion.

In order to implement correctly the analytical properties of the self-energy (Kramers-Kronig, etc.) it is convenient to make a pole expansion,

$$f(\omega) = \sum_n \frac{1}{\omega - \epsilon_n^f - i\delta}.$$

This maps the self-energy to that of an effective Fano-Anderson model of itinerant electrons with conduction bandwidth of order  $t$  which can locally hop onto a distribution of  $f$  levels via a site-dependent hybridization term  $v_r$ . The bath of  $f$  levels simulates the scattering due to the charge fluctuations and provides a Hamiltonian formulation for the self-energy.

We will consider the dynamic case with  $\Delta_r^0 = 0$  and compare with the conventional CDW model ( $v_r = 0$ ,  $\Delta_r^0 \neq 0$ ). A small  $\Delta_r^0$  component added to the frequency dependent case will not change our results significantly. In

addition we will take the modulation to be periodic  $v_r^2 = (1/N_s) \sum_n (v^2)_{n\mathbf{Q}} \exp(in\mathbf{Q} \cdot \mathbf{r})$ . Just as a superconductor with a frequency dependent order parameter has long range off-diagonal order, even with  $\Delta_r^0 = 0$ , the dynamical model has diagonal order given by  $n_r = (1/N_s) \sum_{n,k} \int d\omega \text{Im}G_{\mathbf{k},\mathbf{k}+n\mathbf{Q}} \cos(n\mathbf{Q} \cdot \mathbf{r})$ . In real materials the charge modulations will be linearly coupled to the impurity potentials and the system will easily lose long range order but keeping short range modulations with translational symmetry breaking. This important effect can be incorporated but will be neglected for simplicity.

Motivated by the experiments by Kohsaka *et al.* [16] and previous evidence on stripes [2] we consider a one-dimensional modulation with wave-vector  $|\mathbf{Q}| = 2\pi/4$  along the  $x$  direction. Results for checkerboard patterns will be similar except for the absence of  $C_4$  symmetry breaking. The insets to Fig. 2(a) and 2(b) display the associated modulation  $\Delta_r^0$  and  $v_r^2$ . The resulting charge modulation can be seen as bond-centered (hole) stripes separated by 4 lattice constants, respectively. Our main conclusions do not depend on this particular choice.

The Green function (GF) in  $k$  space can be obtained from the coupled system of equations

$$[\omega - \epsilon_{\mathbf{k}+n\mathbf{Q}} - v_0^2 f(\omega)] G_{\mathbf{k}+n\mathbf{Q},\mathbf{k}+m\mathbf{Q}}^\sigma = \delta_{nm} + \sum_{p \neq n} [\Delta_{(p-n)\mathbf{Q}}^0 + (v^2)_{(p-n)\mathbf{Q}} f(\omega)] G_{\mathbf{k}+p\mathbf{Q},\mathbf{k}+m\mathbf{Q}}^\sigma \quad (2)$$

where the dispersion  $\epsilon_{\mathbf{k}}$  is measured with respect to the chemical potential. While the zero momentum component of the static CDW order parameter  $\Delta_{\mathbf{q}=0}^0$  gets trivially reabsorbed in the chemical potential the same does not occur with the dynamical part. That is  $\Sigma_0^{\text{CDW}}(\omega) \equiv v_0^2 f(\omega)$ , with  $v_0^2 \equiv (v^2)_{\mathbf{q}=0}$ , has to be explicitly taken into account as can be seen from the mapping to the Hamiltonian structure which guarantees the preservation of sum rules for the spectral function. Furthermore, as discussed above, we are forced to take  $v_r^2 \geq 0$  which implies that the Fourier component  $v_0^2$  has to be positive for any nonzero modulation. Thus we have the surprising result that the dynamical CDW scattering produces a momentum independent scattering rate. For a given amplitude of modulation, there is a lower bound for such a scattering rate which is determined by taking the smallest  $v_r^2$  to be zero. This leads to a scattering rate of the charge carriers by the CDW fluctuations  $\Gamma_\omega^{\text{CDW}} \sim \text{Im}\Sigma_0^{\text{CDW}}(\omega)$ . In the following we make this minimum choice which makes  $\Gamma_\omega^{\text{CDW}}$  to be explicitly determined by the sum of amplitudes of the electronic inhomogeneity  $\sim v_0^2$ . Such an intrinsic relation between electronic inhomogeneity and inelastic scattering rate has been recently revealed by STM experiments on Bi2212 materials [14] where it has been shown that the LDOS spectra can be parametrized based on a model with SC  $d$ -wave order supplemented by an energy dependent scattering rate  $\Gamma_\omega^{\text{LDOS}} = \alpha\omega$ . The parameter  $\alpha$  varies spatially and in the regions with pronounced charge order acquires values up to  $\alpha \approx 0.4$ . Also ARPES spectra

[17,18] from Bi2212 materials suggest a marginal Fermi-liquid (MFL) type self-energy (i.e.,  $\text{Im}\Sigma \sim \Gamma_\omega^{\text{ARPES}} \sim \omega$ ) which is increasing with underdoping similar to  $\Gamma_\omega^{\text{LDOS}}$ . Motivated by these experimental findings we describe the CDW dynamics (and therefore  $\Gamma_\omega^{\text{CDW}}$ ) by a marginal Fermi-liquid (MFL) type form [19]

$$f(\omega) = 2\omega \ln \frac{\Gamma + i\omega}{\Omega} + i\pi\Gamma, \quad (3)$$

where  $\Gamma = kT$  corresponds to a temperature scale and  $\Omega$  denotes an upper cutoff of the boson spectrum from which the MFL self-energy is derived [20]. The amplitudes of the charge modulation are chosen such that  $v_0^2 = 0.08$  eV which yields  $\text{Im}\Sigma(\omega) = v_0^2 \text{Im}f(\omega) \approx 0.25|\omega|$  at small frequencies which is close to the average  $\Gamma_\omega^{\text{LDOS}}$  observed. The dispersion  $\epsilon_{\mathbf{k}}$  includes hopping to nearest ( $\sim t_1 = 250$  meV) and next-nearest ( $t_2 = -0.4t_1$ ) neighbors as appropriate for Bi2212 materials.

Figure 1(b) demonstrates that for the dynamic case quasiparticles around the Fermi energy are protected from the CDW scattering. In contrast, static CDW order [cf. Fig. 1(a)] produces the usual FS reconstruction, i.e., flattening of the dispersion around  $(\pi, 0)$  and gap formation between the nodes and  $(0, \pi)$  due to nesting. At higher energies the effect of the dynamic scattering on the spectral function is similar to that of a static CDW, with an additional broadening due to the imaginary part of the self-energy which is increasing with frequency.

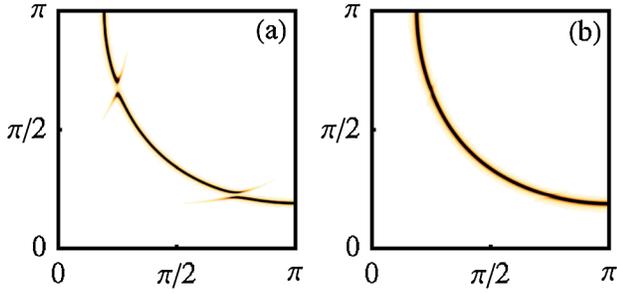


FIG. 1 (color online). Density plots of the integrated spectral weight in a window of  $\pm 5$  meV around  $E_F$ . (a) static CDW with  $\Delta_2^0 - \Delta_1^0 = 0.054$  eV (cf. inset to Fig. 2). (b) dynamic CDW ( $\Delta_i^0 = 0$ ); Residual parameters as given in the text.

As mentioned above the interpretation of STM experiments, which are usually taken at very low temperatures, requires the implementation of superconductivity into the formalism which in Eq. (2) can be added as a BCS-type SC self-energy  $\Sigma_k^{sc} = (\Delta_k^{sc})^2 / [\omega + \varepsilon_k + v_0^2 f^*(-\omega)]$  to the bracket on the l.h.s. Recent STM experiments [21] have revealed that the shape of the tunneling spectra of Bi2212 can be fit by including higher harmonic contributions in addition to the simple  $d$ -wave form. Following this observation we take

$$\Delta_k^{sc} = \sum_n \Delta_0(n) [\cos(nk_x) - \cos(nk_y)] / 2$$

and restrict to the first three harmonics with  $\Delta_0(1) = 40$  meV,  $\Delta_0(2) = -10$  meV, and  $\Delta_0(3) = 5$  meV. For simplicity we take this gap function to be frequency independent.

In Fig. 2 we report the LDOS structure for the model with static (a) and dynamic (b) order parameter including the SC gap. The static order parameter was chosen in order to give a similar magnitude of the intensity difference

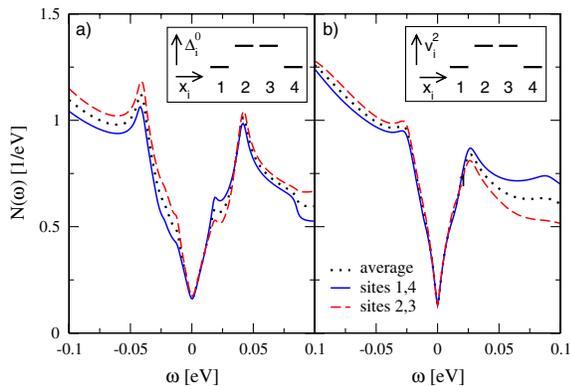


FIG. 2 (color online). LDOS for the model with (a) static CDW scattering ( $\Delta_2^0 - \Delta_1^0 = 0.054$  eV) and (b) frequency dependent CDW scattering. The upper insets depict the modulations of  $\Delta_r^0$  (a) and  $v_r^2$  (b) in the unit cell. Further parameters: chemical potential  $\mu = -0.23$  eV, (doping  $x \approx 0.07$ ),  $\Gamma = 1$  meV, and  $\Omega = 1$  eV.

among different sites (contrast) at high positive bias as the dynamical model.

Because of particle-hole mixing, superconductivity tends to soften the charge order related LDOS modulations at low energies, however the inset in Fig. 3(a) reveals that in the static case substantial residual modulations persist at an energy of  $\omega = \pm 5$  meV specially for negative energies. This contrast is strongly suppressed for the dynamic order parameter [see inset in Fig. 3(b)] as seen experimentally. This is easy to understand due to the structure of  $f(\omega)$  which vanishes at low energies. However, this effect is not very apparent and would hardly allow one to decide for the dynamical model. A much more dramatic difference is instead provided by the sign of the contrast when the bias is reversed. For the static order parameter we observe contrast reversal below the energy of the superconducting gap (i.e., sites with high intensity and low intensity LDOS are inverted when one changes the sign of the bias) while the ordering of the intensities tends to be substantially preserved at high energies (contrast preservation). For the dynamical case the situation is the opposite: there one finds contrast preservation inside and contrast reversal above the superconducting gap. Thus the dynamical model agrees with the ubiquitous contrast reversal found in STM at large energy concomitant with the absence at low energies [15].

How general is this result? In the static case contrast reversal at high energy can be achieved for special situations (e.g., a half-filled system with square Fermi surface, i.e., complete nesting) where asymmetry occurs for higher energies. In these cases the imaginary part of the off-diagonal GF  $\text{Im}G_{k,k+Q}$  has a sign change at the chemical potential since  $k$  states with  $\varepsilon_k < 0$  only connect to  $k + Q$  states above the chemical potential and vice versa. In the case of the dynamical order parameter the sign change has its origin in the dynamical self-energy since  $G_{k,k+Q} \sim f(\omega)$  and  $\text{Re}f(\omega) = -\text{Re}f(-\omega)$  and thus, it does not

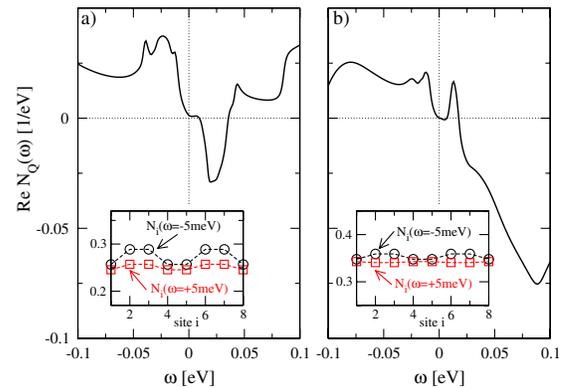


FIG. 3 (color online). Fourier-transformed LDOS at the CDW scattering vector,  $\mathbf{Q} = \frac{2\pi}{4}$ . (a) Static CDW scattering with  $\Delta_2^0 - \Delta_1^0 = 0.054$  eV, (b) frequency dependent CDW scattering. The phase has been chosen such that  $\text{Im}N_{\mathbf{Q}}(\omega) = 0$ . Lower insets: LDOS at  $\omega = +5$  meV (squares) and  $\omega = -5$  meV (circles). Further parameters as in Fig. 2.

require special conditions as nesting. Indeed we have found similar results for other periodicities and fillings.

The oddness of the real part of  $f(\omega)$  is reminiscent of odd frequency superconductors [22]. There however symmetry constrains the oddness to be exact while here it can, in principle, be only approximated as long as  $\text{Im}f(\omega) > 0$ . The hump feature on the positive frequency side of the LDOS in Fig. 2 originates from the nesting of  $\mathbf{Q}$  between the antinodal FS segments. This induces a concomitant increase of the LDOS modulation, which for our underdoped system occurs at energies  $\approx 90$  meV above  $E_F$ .

To analyze the difference between frequency dependent and frequency independent CDW scattering in more detail we show in Fig. 3 the Fourier-transformed LDOS  $\rho(\mathbf{Q}, \omega)$  at the CDW wave vector  $\mathbf{Q} = \frac{2\pi}{4}$ .

As pointed out in Refs. [23,24] the symmetry of the wave-function in a SC with static CDW order implies  $\rho(\mathbf{Q}, \omega) = -\rho(\mathbf{Q}, -\omega)$  for sufficiently small  $\omega$ . In fact, we clearly observe this asymmetry in the LDOS in Fig. 3(a) on the energy scale of the SC gap in contrast to the experimental observation [5] of a symmetric  $\rho(\mathbf{Q}, \omega)$  in this regime. This was explained as due to a modulation of the SC pair density [24,25]. Figure 3(b) shows that the symmetry is also achieved for a dynamic CDW order parameter. Notice that this symmetry can not persist up to high energies since contrast reversal implies that at high energy the dominant Fourier component should change sign. Indeed our dynamic model with  $\Delta^{\text{CDW}}(\omega) \sim f(\omega)$  with  $\text{Re}f(\omega) = -\text{Re}f(-\omega)$  reconciles both aspects, low-energy symmetry of  $\rho(\mathbf{Q}, \omega)$  and a strong high energy odd component leading to contrast reversal.

The present model applies to cuprates where the system at the microscopic scale shows breaking of translational symmetry but sustains low-energy quasiparticles weakly affected by that. A prominent example is  $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$  where a surprisingly well defined Fermi surface has recently been observed [26]. In addition, there are situations with no apparent translational symmetry breaking but with a high energy response resembling that of an ordered system. We have recently presented a scenario for the spectral function in this distinct physical situation [27].

Summarizing, we have presented a simple phenomenological model of a frequency dependent CDW order parameter in cuprates which accounts for the dichotomy between low-energy Bogoljubov quasiparticles and high energy electronically ordered states [13] with the concomitant crossover from LDOS modulations determined from QPI to dynamical CDW scattering at large frequencies. For simplicity we have taken into account a charge order parameter but we expect similar results will apply for a magnetic order parameter. The model has a series of implications which agree with experimental observation: (i) Intimate relation between quasiparticle scattering rate and amplitude of charge order. (ii) Suppression of contrast in the LDOS at low energies. (iii) Contrast reversal

(preservation) at high (low) energies. (iv) Even symmetry of the low-energy Fourier-transformed LDOS. (v) Featureless Fermi surface. While a naive CDW order parameter will be in contradiction with most of these observations the dynamical model reconciles the long suspected charge ordering with these apparently contrasting experiments. Our results for the scattering time suggest to search for the origin of marginal Fermi-liquid behavior in an Eliashberg treatment of charge (and) or spin density waves [28].

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- [1] *Proceedings of the Third Workshop on Phase Separation, Electronic Inhomogeneities and Related Mechanisms in High- $T_c$  Superconductors*, edited by C. Di Castro and E. Sigmund [J. Supercond. 9 (1996)].
  - [2] J.M. Tranquada *et al.*, Nature (London) **375**, 561 (1995).
  - [3] P. Abbamonte *et al.*, Nature Phys. **1**, 155 (2005).
  - [4] J.E. Hoffmann *et al.*, Science **297**, 1148 (2002).
  - [5] C. Howald *et al.*, Phys. Rev. B **67**, 014533 (2003).
  - [6] K. McElroy *et al.*, Phys. Rev. Lett. **94**, 197005 (2005).
  - [7] A. Hashimoto *et al.*, Phys. Rev. B **74**, 064508 (2006).
  - [8] T. Hanaguri *et al.*, Nature Phys. **3**, 865 (2007).
  - [9] W.D. Wise *et al.*, Nature Phys. **4**, 696 (2008).
  - [10] M. Vershinin *et al.*, Science **303**, 1995 (2004).
  - [11] T. Hanaguri *et al.*, Nature (London) **430**, 1001 (2004).
  - [12] Q.H. Wang and D.-H. Lee, Phys. Rev. B **67**, 020511(R) (2003).
  - [13] Y. Kohsaka *et al.*, Nature (London) **454**, 1072 (2008).
  - [14] J.W. Alldredge *et al.*, Nature Phys. **4**, 319 (2008).
  - [15] J.-H. Ma *et al.*, Phys. Rev. Lett. **101**, 207002 (2008).
  - [16] Y. Kohsaka *et al.*, Science **315**, 1380 (2007).
  - [17] T. Valla *et al.*, Science **285**, 2110 (1999).
  - [18] P.D. Johnson *et al.*, Phys. Rev. Lett. **87**, 177007 (2001).
  - [19] P.B. Littlewood and C.M. Varma, J. Appl. Phys. **69**, 4979 (1991).
  - [20] Notice that the definitions of  $\Gamma_{\omega}^{\text{LDOS}}$ ,  $\Gamma_{\omega}^{\text{ARPES}}$ , and  $\Gamma_{\omega}^{\text{CDW}}$  are not the same but are closely related. For example, introducing a MFL form in  $\Gamma_{\omega}^{\text{CDW}}$  automatically generates a MFL in  $\Gamma_{\omega}^{\text{ARPES}}$ . Equation (3) only holds close to the chemical potential whereas the calculation of, e.g., particle numbers requires an appropriate cutoff at higher energies.
  - [21] A. Pushp *et al.*, Science **324**, 1689 (2009).
  - [22] E. Abrahams *et al.*, Phys. Rev. B **52**, 1271 (1995).
  - [23] D. Podolsky *et al.*, Phys. Rev. B **67**, 094514 (2003).
  - [24] H.-D. Chen *et al.*, Phys. Rev. Lett. **93**, 187002 (2004).
  - [25] M. Ichioka and K. Machida, J. Phys. Soc. Jpn. **71**, 1836 (2002).
  - [26] R.-H. He *et al.*, Nature Phys. **5**, 119 (2009).
  - [27] M. Grilli *et al.*, Phys. Rev. B **79**, 125111 (2009).
  - [28] P. Niyaz *et al.*, Phys. Rev. B **48**, 16011 (1993).