LETTER

Paring density waves as the origin of a ring-like RIXS profile in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$

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Keywords: pairing density waves, charge density waves, superconductivity, cuprates, RIXS

Abstract

Density modulations in cuprates are widely believed to be a signature of a charge-density-wave (CDW) order that competes with superconductivity. Recently, we used a weak-coupling approach to claim that these modulations are better accounted by the coexistence of a homogeneous d-wave gap and short-ranged pairing density waves (PDW) [1]. The full momentum dependence of the density waves in Bi$_2$Sr$_2$CaCu$_2$O$_8+\delta$ (Bi2212) was recently explored in a resonant inelastic x-ray (RIXS) experiment that spanned the entire copper-oxide plane [2], in contrast to previous studies which showed only one-dimensional cuts along specific directions. The main result of this experiment was an apparent ‘ring’ charge order in all directions of the copper-oxide plane. Here, we show that our approach captures well this ring-like intensity profile and its correspondence energy dependency. These results are compatible with the interpretation that the density modulations in cuprates have a predominant PDW character.

Almost twenty years ago, scanning tunneling microscopy (STM) experiments found incommensurate density waves on the surface of Bi$_2$Sr$_2$CaCu$_2$O$_8+\delta$ (Bi2212) [3–6]. Ten years later, resonant x-ray scattering experiments detected a similar incommensurate order in the bulk of YBa$_2$Cu$_3$O$_{7-\delta}$ (YBCO) [7–9]. The same order was later found in a large number of cuprates, demonstrating that this effect is ubiquitous [10–29]. A common approach claims that these modulations are due to a charge density wave (CDW) order that competes with superconductivity. In a recent publication [1], we claimed that short-ranged pairing density waves (PDW) within a d-wave superconducting phase are the correct interpretation of the experimental results. Using a weak-coupling approach, we demonstrated that PDWs and CDWs lead to distinctive momentum and energy dependencies: for PDW the scattering signal peaks at momentum $(\pm q, 0)$, $(0, \pm q)$, while for CDW it peaks at $(0, 0)$. In addition, the PDW signal is expected to be mainly elastic $\Omega = 0$, in contrast to the CDW case, where the signal is expected to peak at $\Omega = \pm 2\Delta_0$. The experimentally detected signal is peaked at $(\pm q, 0)$, $(0, \pm q)$ and at energy $\Omega = 0$, indicating that the observed density waves have a predominant PDW nature.

Recently, a state-of-the-art experiment was performed using resonant inelastic x-ray scattering (RIXS), spanning the entire copper-oxide plane of Bi2212 [2]. The main result was the existence of an inelastic ring-like intensity peak in the $q_x - q_y$ plane with a radius of $q \approx 0.27$ rlu, and with an enhanced signal along the $(\pm q, 0)$ and $(0, \pm q)$ directions. The authors attempted to explain this signal by considering the Coulomb interaction between valence electrons, with short and long-range contributions, but concluded that this explanation is insufficient to account for the full intensity profile. In addition, motivated by the fact that the quasi-elastic ($200 < \Omega < 200$ meV) intensity is more strongly peaked at $(\pm q, 0)$, $(0, \pm q)$ with respect to the higher energy signal ($500 < \Omega < 900$ meV), they suggested a scenario of static directional CDW, combined with dynamic fluctuating ones. To account for these fluctuations, the authors considered the effect of the dynamic susceptibility, characterized by the Lindhard function. However, as they showed in the Supplementary Material.
(Note 5), this approach mainly yields peaks in the wrong direction - $(\pm q, \pm q)$ - and has a square-like shape unlike the smooth ring shape observed in the experiment.

Although we agree that this form of the Lindhard function (which was first suggested as an explanation for resonant x-ray experiments by us in [30]) fails to provide the correct profile of the intensity, we believe that the authors’ choice to discard Fermi-surface effects is incorrect. Indeed, if the observed signal is due to PDW fluctuations, rather than CDW ones, one needs to compute the response from a pairing-like impurity in the presence of a constant d-wave pairing gap [1]. The Born approximation leads to the density response

$$\chi(q, \Omega) = \int d\omega \int d^dk \text{Tr}[G_0(k, \omega)V_k G_0(k + q, \omega + \Omega)\sigma^\dagger].$$

(1)

Here, $V_k = \Delta_k \sigma^x$ models the impurity, $\sigma^j$ are Pauli matrices, $\Delta_k = 0.5\Delta_0(\cos(k_x) - \cos(k_y))$ is the pairing gap and $G_0(k, \Omega) = (-\omega\sigma^0 + (\xi_k - \mu)\sigma^z + \Delta_k \sigma^x)^{-1}$ is the bare Green’s function, where $\xi_k$ is the band structure of the material, and $\mu$ the chemical potential. By performing the integral over $\omega$, one obtains

$$\chi(q, \Omega) = \int d^dk \frac{2\pi \Delta_k (\xi_k \Delta_{k+q} + \xi_{k+q} \Delta_k)}{(E_k - E_{k+q})^2 + (\Omega - i\Gamma)^2}\left(\frac{1}{E_k} - \frac{1}{E_{k+q}}\right).$$

(2)

where $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ and $\Gamma$ is set by the maximum between the quasiparticles’ inverse lifetime and the experimental energy resolution. This approach leads to a strong peak in the $(\pm q, 0)$, $(0, \pm q)$ direction, along with weaker maxima in the diagonal directions (see figure 2 of [1]). In [1] we considered a minimal model of the Fermi surface, where the band structure includes only nearest- and next-nearest-neighbor hopping, highlighting the generality of the results.

In this Letter, we show that the experimental signal of reference [2] can be reproduced without invoking dynamical electronic correlations, by considering a realistic Fermi surface that includes longer-range couplings. Specifically, we use here the phenomenological band structure of Bi2212 proposed by reference [31]:

$$\xi_k = 0.5t_0(\cos(k_x) + \cos(k_y)) + t_1 \cos(k_x) \cos(k_y) + 0.5t_2(\cos(2k_x) + \cos(2k_y)) + 0.5t_3(\cos(2k_x) \cos(k_y) + \cos(2k_y) \cos(k_x)) + t_4 \cos(2k_x) \cos(2k_y),$$

with $t_0 = -0.5951 eV$, $t_1 = 0.1636 eV$, $t_2 = -0.0519 eV$, $t_3 = -0.1117 eV$, $t_4 = 0.510 eV$. The chemical potential $\mu$ is fixed by the doping through the Luttinger count, and the only free parameters are $\Delta_0$ and $\Gamma$, which we set to the experimentally relevant values of $\Delta_0 = 0.1 eV$ and $\Gamma = 0.001 eV$.

This band structure models the bonding Fermi surface: the anti-bonding surface is either very close to the bonding one [32], or characterized by a smaller nesting vector, which is inconsistent with the experimental observations.

Our main results are presented in figure 1, where the two top panels show, respectively, the phenomenological Fermi surfaces and the elastic component ($\Omega = 0$) of the predicted RIXS signal, equation (2), for different doping levels. In these plots, one observes the known PDW signal at the $(\pm q, 0)$, $(0, \pm q)$ directions, accompanied by weaker peaks at $(\pm q, \pm q)$. These peaks can be interpreted as weak CDW modulations, born from the interplay between the static d-wave order and the short ranged PDW [1].

In the lower panel of figure 1, we address the frequency dependence of the RIXS signal. This signal derives from an exchange of energy between the incoming photons and the electrons, whose microscopic description has been studied in detail (see references [33, 34] for a review). In Reference [1] we proposed a phenomenological description of the energy dependence of RIXS experiments by evaluating equation (2) at finite $\Omega$. In the lowest panel of figure 1 we plot $|\chi(q, \Omega)|$ at $\Omega = 0.7 eV$, which is in the middle of the high-energy window of reference [2]. These plots closely resemble the experimental observations at high energy scales, where the peaks at $(\pm q, 0)$ and $(0, \pm q)$ become less pronounced and a clear ring is apparent.

Importantly, for overdoped samples in the high-energy regime, CDW leads to larger contribution with respect to PDW, due to the dispersive nature of the latter, which causes a broadening of the signal [1]. In addition, in these samples the nesting areas in the Fermi-surface become less parallel, further reducing the PDW contribution. This last effect can be more clearly seen in figure 2, where we show the energy dependence of the signal for a one dimensional cut along the $(q, 0)$ direction. As the energy increases, the strong quasi-elastic peak (between $-200$ and $200$ eV) centered around $\Omega \approx 0$ and $q_k \approx 0.3$ rlu is substituted by a dispersive signal which shifts towards larger $q$ and becomes weaker, with increasing doping.

In summary, our numerical calculations show that, in contrast to the interpretation provided in reference [2], the experimental observations are consistent with the known Fermi surface of Bi2212, provided that PDW, rather than CDW, oscillations are considered. It is important to note here that an inelastic signal (at lower frequencies around the mid-IR) along the $(q, q)$ direction was found in other cuprates, such as Hg1201 [35] and electron-doped NCCO [26] (recently also in Bi2212'). These findings are compatible with our conclusion that the observed modulations are a general feature of cuprates based on their band structure. We note that this

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\footnote{The Matlab code used to produced the elastic and energy-resolved maps can be found here available online at \url{stacks.iop.org/JPCO/5/101001/mmedia}.}

\footnote{Between 0.1–0.5 eV. Riccardo Arpaia (private communication).}
model can, in principle, be generalized to take into account the superconducting response as reflected in STM experiments with superconducting tips, whose energy and momentum dependence shows an even richer phenomenology [36]. As for RIXS, our results calls for a further investigation of this signal, with better energy resolution and in the presence of a magnetic field, to refine our understanding of the precise nature of these modulations.

**Acknowledgments**

This work is supported by the Israel Science Foundation Grants No. 967/19, No. 151/19 and No. 154/19.
Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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