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Pairing modulations and phase separation instabilities in $Bi_2Sr_2CaCu_2O_{8+\delta}$

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ABSTRACT

There is growing evidence that the unconventional spatial inhomogeneities in the doped high-T_c superconductors are accompanied by the pairing of electrons, subsequent phase transitions and condensation into coherent states. We show that such pairing states can be obtained from phase separation instabilities near level crossings. Conditions for coherent pairing instabilities are examined using exact diagonalization of Hubbard-like pyramid structures under variation of coupling and interaction strengths. We also evaluate the behavior of the energy charge gap in the vicinity of level crossings using a parametrization of coupling to the apical site to represent out-of-plane effects. These results provide a simple microscopic explanation of (correlation induced) supermodulation of the coherent pairing gap observed in scanning tunneling microscopy measurements at atomic scale in $Bi_2Sr_2CaCu_2O_{8+\delta}$.

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1. Introduction

In spite of intense theoretical and experimental studies there is still no a consensus on the mechanism and origin of the high-T_c superconductivity since the discovery of phenomenon observed first in cuprates almost three decades ago. Recently, the progress has been made due to the new state of the art experimental tools such as scanning tunneling spectroscopy (STM) that provides detailed atomic imaging on the local electronic state. High resolution atomic probe is crucial for observations of nanoscale electronic inhomogeneities which can influence the superconducting electronic structure at the atomic scale. In addition, there have been significant efforts focused on the out-of-plane effects in the cuprate high T_c superconductors (HTSCs), since all the cuprate families share the same CuO_2 plane, but the maximum T_c varies dramatically from one cuprate family to another [1]. This variation is unlikely to be caused by the electronic interactions in the CuO_2 plane alone, but it is mostly due to different layered structures between the CuO_2 planes and their indirect effect on the electronic structure in the CuO_2 plane.

Because of the natural cleavage plane between two BiO layers, $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) system has been ideal for probing the planar electronic structure. This material has a complicated superstructure modulation (supermodulation) which is known to have a strong effect on the position of the apical oxygens but almost no effect on the CuO_2 plane [2,3]. Slezak et al. measured the local superconducting gap using STM with atomic precision and found that the energy gap has a modulation with the same periodicity as the structural supermodulation [4]. Recently, it has been argued that the non-planar apical oxygen atoms in the CuO_5 pyramid or CuO_6 octahedron play an important role in the out-of-plane atomic-scale effects in HTSCs [1,5–7].

In attempts to understand HTSCs, many theoretical models focus only on the planar geometry. However, out-of-plane effects are obviously relevant to the superconducting transition temperatures as these vary significantly among various classes of high temperature superconductors. This suggests that the position of apical atoms or the neighboring layers to the CuO_2 planes are essential in controlling in-plane hole density, i.e., electron pairing. Slezak et al. showed a direct link between the spatial modulation of the out-of-plane atomic structure within an individual unit cell and the variation of the local gap maximum [4]. The non-planar atoms, especially the apical oxygen atoms, are playing an indirect but important role on modulating the local electronic structure of the CuO_2 plane. From their X-ray absorption spectroscopy, Merz et al. [6] concluded that increasing O dopants can induce holes on both oxygens in the CuO_2 plane and the apical oxygen atom. This result suggests that both the planar and (out-of-plane) apical sites

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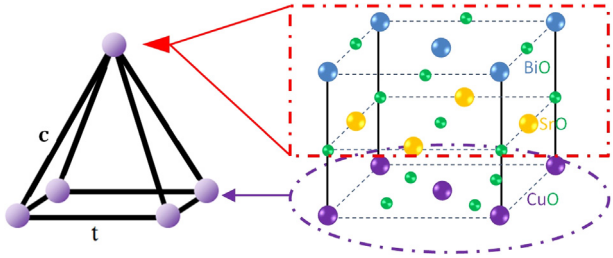

Fig. 1. A schematic picture of the square pyramid structure discussed in the text with an approximate visual aid indicating the attempted connection to the real crystal structure: in particular, at this approximate level, the apical site in the pyramid is expected to represent all the out-of-plane effects in the real crystal following Ref. [4]. The hopping parameters on the basal plane are denoted by t and the hopping parameter c $(= t_i')$ between the apical and basal sites can be independently varied.

can be electronically connected and might be controlling the local electronic state by exchanging holes between the CuO_2 plane and other planes. This could be the origin of interlayer couplings and local gap variations. Therefore, in order to simulate the spatial gap modulation, we need a model that can treat the local electronic correlations accurately while including out-of-plane layered structures that can exchange electrons/holes with the basal atoms. One simple and straightforward way to deal with this is to use Hubbard-like pyramid structures to probe local correlations and an extra out-of-plane site to control the electron/hole concentration on the CuO_2 plane.

Small Hubbard cluster studies, based on exact diagonalization, have provided some important insights into pairing and phase separation instabilities (with local inhomogeneities) [8,9]. When local correlations play a central role in giving rise to an electron instability, these may survive changes in cluster size and boundary conditions, but not geometry/lattice coordination. One is therefore led to believe that there is some essential physics that remains invariant over several classes of high temperature superconductors. An effective attractive interaction resulting from purely electronic means has been found in Betts square unit cells which are said to be ideal for releasing frustration (Ref. [10]). This attraction leads to an instability in electron density distribution in the many-body electronic structure due to level crossing. Clearly, being close to a state with local antiferromagnetism seems to be a necessary condition for stability of pairing. However, it must be noted that we are not in a position to model a single apical oxygen atom; what we can do is accommodate the collective, out-of-plane effects in a dressed-site that acts like a reservoir by supplying electrons or holes to the planar sites. This coupling and its on-site repulsion can be utilized as independent parameters that are expected to mimic the behavior of the pairing gap and its dependence on the coupling to the out-of-plane sites.

The paper is organized as follows: Following the introduction to various aspects of pairing modulations, we present our microscopic model and methodology of exact cluster calculations of pyramidal structures in Sections 2 and 3. In Section 4, we show the results of charge gap variations and comparisons with pairing modulation in $Bi_2Sr_2CaCu_2O_{8+\delta}$. The concluding summary constitutes Section 5.

2. Model

To address an atomic-scale physics we begin with the canonical Hubbard-like model on a square pyramid unit cell consisting of five atoms, i.e., $L = 5$ (as shown in Fig. 1).

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(c_{i\sigma}^{+} c_{j\sigma} + \text{H.c.}\right) - \sum_{i,\sigma} \left(t_i' a_{\sigma}^{+} c_{i\sigma} + \text{H.c.}\right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + U_{apical} n_{a\uparrow} n_{a\downarrow}. \quad (1)$$

Here, $c_{i\sigma}$ $(c_{i\sigma}^{+})$ is the electron destruction (creation) operator at the basal sites with spin σ with the total electron number at the basal plane, $N_{basal} = \sum_{i\sigma} n_{i\sigma}$, while a_{σ} (a_{σ}^{+}) is the same operator at the apical site with $N_{apical} = n_{a\uparrow} + n_{a\downarrow}$ correspondingly. The first term indicates the hopping between the nearest (intra-plane) basal sites. The second term describes interlayer coupling between the apical and basal sites i with a hopping parameter t_i'. In addition, $U > 0$ is the on-site Coulomb interaction at the basal sites i while at the apical site, we have the freedom to choose a different $U_{apical} > 0$. The cluster can be solved exactly for all the eigenvalues and eigenvectors [11]. The apical site can exchange electrons/holes with all the basal sites; i.e., displacements in position can affect the planar electronic structures and promote the change of electron configuration on apical site associated with the out-of-plane layers.

In non-bipartite structures, such as the pyramid or tetrahedron, the electronic structure depends strongly on the sign of t and c. Here the pyramidal non-bipartite geometry is defined by choosing $t > 0$ as the hopping parameter connecting the (plaquette) sites in the square basal plane. The parameter $c > 0$ can closely imitate the interlayer coupling response in multilayer structures (see Fig. 1). Also, all the energy parameters are measured in units of t, unless otherwise stated.

3. Methodology

An essential element for understanding our results on pairing modulation is the formation of a coherent pairing state of N electrons having a negative charge gap and a positive spin gap obtained previously in Refs. [8–14] and references therein. For completeness, here we first briefly summarize the key results of exact diagonalization in small clusters at weak and moderate U values. The results from square lattices, generated recently from optimized (finite) Betts unit cells (Ref. [10]), provide strong support for the phase separation instabilities found in generic coupled (square) clusters [9,14]. Betts cells are believed to alleviate frustrations due to various size effects. In addition, our Variational Cluster Approach (VCA) based work, which incorporates long range effects through extrapolations to larger systems, provides further support that such instabilities do prevail in larger lattices [15]. One note of caution: *Many recent STM studies [16–20] seem to suggest that the gap detected by them is the so-called pseudogap, although the early work of Slezak [4] identified it as the superconducting gap. In view of the controversy over the interpretation of the pseudogap, we will only focus on what we would clearly define as the pairing gap, therefore, making no attempt to compare our results outside the optimally doped regime.*

3.1. Charge and spin gaps

Numerical (exact) calculations of the many-body energy levels, E_n, for the relevant total electron number $N = N_{apical} + N_{basal}$ and a total spin $S = S_{apical} + S_{basal}$ are used to define charge and spin gaps. Here, we focus on one hole off half-filling case (optimal doping), when total number of electrons is fixed to $L - 1$, i.e., $\langle N\rangle = 4$. The charge excitation gap Δ^c at finite temperature can be written as an energy difference of canonical energies, $\Delta^c(N,T) = \mu_+ - \mu_-$, where $\mu_+ = E_{N+1}(T) - E_N(T)$ and $\mu_- = E_N(T) - E_{N-1}(T)$. The charge gap determines the stability of an N-electron state with the density $n = N/L$ compared to an equal admixture of $(N+1)$- and $(N-1)$-electron states (the average number of electrons for this mixture is still n). Depending on the strength of the on-site electron–electron repulsion U, this charge excitation gap can be positive $\Delta^c > 0$ or negative $\Delta^c < 0$. The pair binding energy $\Delta^c(N,T)$ determines whether a total of $2N$ electrons in a pair of isolated clusters prefer to be distributed uniformly $(\Delta^c > 0)$ or