

Puzzles about 1/8 magic doping in cuprate

D.L. Feng^a, Z.-X. Shen^{b,*}, X.J. Zhou^b, K.M. Shen^b, D.H. Lu^b, D.v.d. Marel^c

^a Applied Surface Physics State Key Laboratory, Department of Physics, and Synchrotron Radiation Research Center, Fudan University, Shanghai 200433, China

^b Applied Physics and Stanford Synchrotron Radiation Laboratory, Department of Physics, Stanford University, Stanford, CA 94305, USA

^c Département de Physique de la Matière Condensée, Université de Genève, CH-1211 Geneva 4, Switzerland

Abstract

We discuss the puzzles surrounding the interpretation of the 1/8 anomaly in cuprates, highlighting the tension between the real and reciprocal space ways to look at the problem. This issue is relevant to the current discussion on the nature of charge ordering in the form of ‘stripe’ and ‘checker-board’ as derived from neutron and STM experiments. A resolution of this tension is important to fully understand the electronic structure.

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An interesting phenomenon in the cuprates is the 1/8 anomaly where the superconducting transition temperature is suppressed [1–4]. This effect is usually attributed to the formation of stripes. In this picture, the stripes are half-filled, i.e. one of the two sites on the stripes is filled with an electron (Fig. 1) [5]. The 1/8 anomaly corresponds to the situation when three insulating lines exist between the metallic stripes, thus there is one hole per eight sites. The anomaly in this case is presumably related to the commensurability of this stripe configuration with the underlying lattice. This interpretation, together with the interpretation of the neutron scattering data [5], makes a self-consistent picture.

While attractive, some questions remain in this interpretation of the 1/8 anomaly. For example, one would expect 1/10 or 1/6 doping to be an anomaly too. The counting of holes at 1/8 doping and its commensurability with the lattice would work only in the model where the charge modulation between the metallic stripes and the insulating regions around them is strong as in the cartoon of Fig. 1, something yet to be established. Finally, it is unclear why the stripes should be half-filled. Before these questions are satisfactorily addressed, it is reasonable to ask whether any other approach may also produce the magic number of 1/8 doping.

In this short paper, we wish to point out that if the Fermi surface has the approximate shape containing the shaded cross-region in Fig. 2, which may provide another way to look at the 1/8 anomaly. In this case, the Fermi

surface consists of two parallel sections separated by $2\pi/4a$. This, of course, is a highly idealized picture just like the idealized model of Fig. 1, an issue which we will discuss later. For now, we proceed to show for such a Fermi surface that, if it is assumed to have an instability when it is incommensurate with the underlying lattice, it produces a series of magic numbers, with 1/8 falling inside the experimentally allowed doping range.

Taking the separation between two straight Fermi surface segments as a fraction ν of the entire Brillouin zone and assuming for the moment that the Fermi surface is indeed as perfectly crossed as indicated by the edge of the shaded region in Fig. 2, then the occupied part of the Brillouin zone is

$$N = 2\nu - \nu^2$$

The number of electrons per unit cell equals $2N$ due to spin degeneracy, and the doping of the cuprates is counted from half-filling, hence

$$x = 1 - 2N = 1 - 4\nu + 2\nu^2$$

When the Fermi surface nesting is commensurate with the lattice, where the charge density wave (CDW) instability is the strongest, $\nu = 1/n$ with n being an integer. We have

$$x = (2 + n^2 - 4n)/n^2$$

and, substituting $n=4, 5, 6\dots$ the following series of ‘magic’ fractions is obtained

$$x = \frac{1}{8}, \frac{7}{25}, \frac{7}{18}, \frac{23}{49}, \dots$$

* Corresponding author.

E-mail address: zxshen@stanford.edu (Z.-X. Shen).

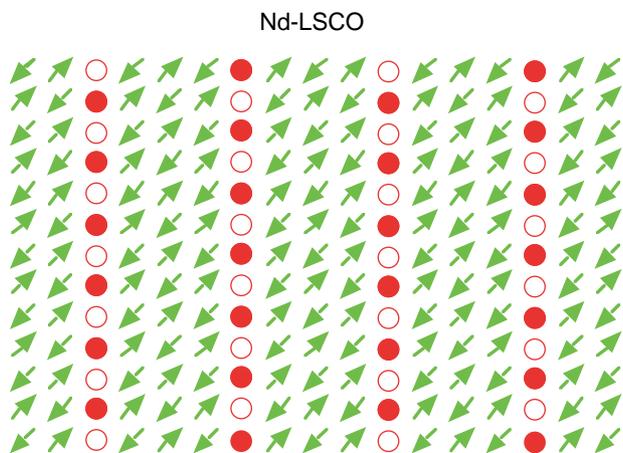


Fig. 1. Cartoon picture of vertical stripes in Nd-LSCO at 1/8 doping as proposed in Ref. [5]. The arrow represents the spins between the stripes. The empty circle represents the hole and the filled circle represents an electron with uncertain spin orientation.

for hole doping. So far, only crystals with the first two magic dopings $x=0.125$ and $x=0.28$ have been prepared in the hole doped materials. As 0.28 hole doping is near the boundary of the superconducting phase anyway, 1/8 is the only magic doping number in the realistic range. The CDW at 1/8 doping, without invoking the half-filled stripes scenario, could give similar Bragg peaks as observed in $\text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4$ (Nd-LSCO) by neutron scattering experiments [5].

In $\text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4$, parallel ‘Fermi surface’ sections with $\pi/4$ separation has been experimentally observed in the $n(\vec{k})$ data near 1/8 doping [7]. However, caution should be taken as the results near the anti-node change with photon energy [8]. This change is probably related to the k_z effect which is found to strongly influence the anti-nodal region [9], where a weak in-plane band dispersion and an enhanced k_z dispersion complicate the situation. Straight Fermi surface segments have also been observed near the anti-nodal region by

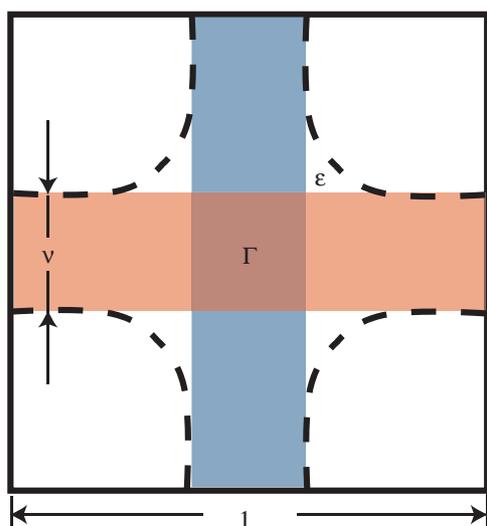


Fig. 2. Typical Fermi surface of cuprates in the first Brillouin zone [6]. All numbers are in the unit of $2\pi/a$.

angle resolved photoemission spectroscopy (ARPES) experiments in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi2212), $\text{Bi}_2\text{Sr}_2\text{CuO}_{6+\delta}$ (Bi2201) and $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+\delta}$ (LSCO) systems from the underdoped regime up to the slightly overdoped regime [8,10–13]. These segments are parallel to the (1,0) or (0,1) direction, and are separated from the (1,0) or (0,1) line by about $\pi/4$. More recently, similar straight Fermi surface segments have also been Na-doped $\text{Na}_x\text{Ca}_{2-x}\text{CuO}_2\text{Cl}_2$ (Na-CCOC) systems at $x=0.05, 0.10, 0.12$ [14]. Therefore, the idealized Fermi surface in Fig. 2 does capture some important features of material despite the deviations here and there. Given the broadness of the features in momentum and energy, some Fermi surface related CDW instability is possible, especially when it is commensurate with the lattice. For this reason, the fact that it can give 1/8 magic doping is intriguing.

The reciprocal space picture in Fig. 2 has its own weaknesses. For example, Fermi surface changes with k_z (and thus the photon energy) [9], and the almost perfectly nested Fermi surface in the case of overdoped Bi2212 [13] and Na-doped CCOC does not coincide with a T_c anomaly. More seriously, there are significant nodal states which modify the Fermi surface as illustrated by the dashed line in Fig. 2, where the Fermi surface volume deviates from the perfect cross by 4ϵ as indicated. With a typical value of 4ϵ of 0.04, this makes the magic doping to be different from 1/8.

This brings us to the central dilemma about understanding the ‘magic’ 1/8 doping level and the charge ordering physics in general: these are quite delicate issues, and the lightly idealized pictures in both real space (as in Fig. 1) and in reciprocal space views (as in Fig. 2) have failed to provide a comprehensive understanding, although they do in their own manners give us a way to visualize the physics. The same tension between the real space and reciprocal space views is also clearly at display in our struggle to understand the ‘checker-board’ patterns observed by Scanning Tunneling Microscopy (STM) [15–18]. If one tries to go with the idealized model in real space like a Wigner crystal of charge or charge pairs, it is difficult to rationalize the nodal state that is so dominating even in the charge ordered state [14].

In summary, using 1/8 anomaly as an example, we highlight the tension of real and reciprocal space views of the charge ordered state. Given that our theoretical tools are usually based on these views, we suggest that a resolution of this tension is a key step towards understanding the novel electronic state of cuprates.

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