Spectroscopic Imaging STM studies of broken electronic symmetries in underdoped cuprates

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Abstract. We use spectroscopic imaging scanning tunneling microscopy (SI-STM) to visualize the spatial symmetries of the electronic states that occur at the pseudogap energy scale in underdoped cuprates. We find evidence for the intra-unit-cell electronic nematicity - by which we mean the breaking of C4v symmetry within each CuO2 unit cell[1]. We also find that the coexisting incommensurate (smectic) electronic modulations couple to the intra-unit-cell nematicity through their 2π topological defects[2].

In general for underdoped cuprates, the electronic excitations at the pseudogap energy range $E \sim \Delta_1$ are observed to be highly anomalous. They are associated with a strong antinodal pseudogap in $\vec{k}$-space [3, 4], they exhibit slow dynamics without recombination to form Cooper pairs [5], their Raman characteristics appear distinct from expectations for a d-wave superconductor[6], and they appear not to contribute to superfluid density[7]. The spatial symmetries of these states can be explored using high resolution SI-STM. This approach allows the simultaneous visualization of incommensurate electronic-structure modulations that break translational and rotational symmetry (smectic), and intra-unit-cell electronic structure that does not break translational symmetry but does break rotational symmetry (nematic). The relationship between these electronic phenomena which, because they break different symmetries are distinct, can also be explored directly using this approach. To pursue these objectives, we have introduce several new SI-STM techniques [1],[2].

We measure the differential conductance $g(\vec{r}, E) = \frac{dI}{dV}(\vec{r}, E = eV)$ simultaneously with topograph $T(\vec{r})$ on the Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ surface. In order to characterize the correct symmetry of the electronic structure, we use $Z(\vec{r}, E) \equiv \frac{g(\vec{r}, E=+eV)}{g(\vec{r}, E=-eV)}$ in which potentially severe systematic errors are effectively cancelled[9, 10]. Atomically resolved $\vec{r}$-space images of the static phenomena in $Z(\vec{r}, E)$ show highly similar spatial patterns at all energies near $\Delta_1$ but with variations of intensity due to the $\Delta_1$-disorder[10]. By changing to reduced energy variables...
The magnitude of $O$ over the entire field of view (FOV) as a function of the average throughout Fig.1b. We defined a normalized measure of intra-unit cell $T$, the $Z$ within the unit cell to at least $180^\circ$ break translational symmetry, and reduce the expected $90^\circ$ maximum in intensity at $e = 1[9]$. Thus the pseudogap states of underdoped cuprates locally break $C_4$ symmetry[9, 10], and possibly to an even lower symmetry.

To explore which spatial symmetries are actually broken by the cuprate pseudogap states, we use sub-unit-cell resolution imaging performed on multiple different underdoped \(\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}\) samples with $T_c$s between 20K and 55K. The necessary registry of the Cu sites in each $Z(\vec{r}, e)$ is achieved by a picometer scale transformation which renders the topographic image $T(\vec{r})$ perfectly $a_0$-periodic[1]; the same transformation is then applied to the simultaneously acquired $Z(\vec{r}, e)$ to register all the electronic structure data to this ideal lattice. The topograph $T(\vec{r})$ is shown in Fig.1a; the inset compares the Bragg peaks of its real (in-phase) Fourier components $\text{Re} T(\vec{Q}_x)$, $\text{Re} T(\vec{Q}_y)$ and demonstrates that $\text{Re} T(\vec{Q}_x)/\text{Re} T(\vec{Q}_y) = 1$. Therefore $T(\vec{r})$ preserves the $C_4$ symmetry of the crystal lattice. In contrast, Fig.1b shows that the $Z(\vec{r}, e = 1)$ determined simultaneously with Fig.1a breaks various crystal symmetries[1]. The inset shows that since $\text{Re} T(\vec{Q}_x)/\text{Re} T(\vec{Q}_y) \neq 1$ the pseudogap states break $C_4$ symmetry on the average throughout Fig.1b. We defined a normalized measure of intra-unit cell $C_2$ symmetry over the entire field of view as a function of $e$:

$$O_N^Q(e) \equiv \frac{\text{Re} Z(\vec{Q}_y, e) - \text{Re} Z(\vec{Q}_x, e)}{Z(e)}$$

(1)

where $Z(e)$ is the spatial average of $Z(\vec{r}, e)$. The plot of $O_N^Q(e)$ in Fig.1c shows that the magnitude of $O_N^Q(e)$ is low for $e \ll \Delta_0/\Delta_1$, begins to grow near $e \sim \Delta_0/\Delta_1$ , and becomes well defined as $e \sim 1$ or $E \sim \Delta_1(\Delta_0)$ is defined as a kink in local density of states[8]).

To explore a source for these effects within the CuO$_2$ unit cell, we study with sub-unit-cell resolution. Fig.1d shows the topographic image of a representative region from Fig.1a; the locations of each Cu site $\vec{R}$ and of the two O atoms within its unit cell are indicated. Fig.1e
shows measured simultaneously with Fig.1d with same Cu and O site labels. Next we define

\[ O_N^R(e) = \sum_{\vec{R}} \frac{Z_x(\vec{R}, e) - Z_y(\vec{R}, e)}{Z(e)N} \]

where \( Z_x(\vec{R}, e) \) is the magnitude of \( Z(\vec{r}, e) \) at the O site \( a_0/2 \) along the \( x \)-axis from \( \vec{R} \) while \( Z_y(\vec{R}, e) \) is the equivalent along the \( y \)-axis, and \( N \) is the number of unit cells. This is the \( r \)-space measure of \( C_2 \) symmetry is equivalent of \( O_N^Q(e) \) in Eqn.1 but counting only O site contributions. Fig.1e contains the calculated value of \( O_N^S(e) \) from the same FOV as Fig.1a,b revealing the good agreement with \( O_N^S(e) \).

For all samples studied, the low values found for at low \( e \) occur because these states are dispersive Bogoliubov quasiparticles[11, 10] and cannot be analyzed in term of any static electronic structure, smectic or otherwise. More importantly \( |O_N^Q(e)| \) shows no tendency to become well established at the pseudogap or any other energy[1].

To visualize the separate broken symmetries in the \( E \sim \Delta_1 \) electronic structure, we consider \( Z(\vec{q}, e = 1) \) in Fig.2a inset; this is the Fourier-space representation of electronic structure of the \( E \sim \Delta_1 \) states. Taking into account only the Bragg peaks at \( \vec{Q}_x, \vec{Q}_y \) (red circles/arrows in Fig.2a inset) the coarse grained image of \( C_4 \) symmetry breaking at \( \vec{Q} = 0 \) intra-unit-cell electronic structure is revealed as shown in Fig.2b. By contrast, if one focuses upon the incommensurate modulations \( \vec{S}_x, \vec{S}_y \) (blue circles/arrows in Fig.2a), we find a disordered electronic structure which breaks both \( C_2 \) and translational symmetry locally as shown in Fig.2c. Although these two types of electronic phenomena represent clearly distinct broken symmetries, SI-STM reveals that they coexist in the \( E \sim \Delta_1 \) pseudogap electronic structure of underdoped cuprates[1].

The distinct properties of the smectic electronic structure modulations at \( E \sim \Delta_1 \) can be examined independently of the intra-unit-cell symmetry breaking by focusing only upon the incommensurate modulation peaks \( \vec{S}_x \) and \( \vec{S}_y \). A coarse grained image of the local smectic symmetry breaking (Fig.2c) reveals the very short correlation length of the strongly disordered smectic[9, 10]. The amplitude and phase of two unidirectional modulation components (along \( x, y \)) within box in Fig.2a can be further extracted as shown in Figs.3a,b[2]. To do so, we denote the local contribution to the \( \vec{S}_y \) modulations at position \( \vec{r} \) by a complex field \( \Psi_1(\vec{r}) \). This contributes to the \( Z(\vec{r}, e = 1) \) data as \( \Psi_1(\vec{r})e^{i\vec{S}_x\cdot\vec{r}} + \Psi_1^*(\vec{r})e^{-i\vec{S}_x\cdot\vec{r}} \equiv 2|\Psi_1(\vec{r})|\cos(\vec{S}_x\cdot\vec{r} + \phi_1(\vec{r})) \) thus allowing the local phase \( \phi_1(\vec{r}) \) of \( \vec{S}_x \) modulations to be mapped; similarly for the local phase \( \phi_2(\vec{r}) \) of the \( \vec{S}_y \) modulations. In Figs.3c,d we show images of \( \phi_1(\vec{r}) \) and \( \phi_2(\vec{r}) \) derived from \( Z(\vec{r}, e = 1) \). They reveal that the smectic phases \( \phi_1(\vec{r}) \) and \( \phi_2(\vec{r}) \) take on all values between 0 and \( \pm 2\pi \) in a highly complex spatial pattern. Even more significant is the observation of large numbers of topological defects with \( \pm 2\pi \) phase winding. These are indicated by black (\( +2\pi \)) and white (\( -2\pi \)) circles in Figs.3c,d and occur in approximately equal numbers. A typical example
of an individual topological defect is seen in the solid box in Fig.3a and 3c. The dislocation core and its associated $2\pi$ phase winding are clearly seen. Moreover the amplitude of $\Psi_1(\vec{r})$ or $\Psi_2(\vec{r})$ always goes to zero near each topological defect. These data are all in excellent agreement with the theoretical expectations for quantum smectic dislocations (Fig.2c inset).

Imaging the locations of topological defects (Figs.3c,d) with the intra-unit-cell nematicity (Fig.1b) reveals another key result. Fig.3e shows the locations of all topological defects in Figs.3c,d plotted as black dots on the simultaneously obtained $\delta O_N(\vec{r}) = O_N(\vec{r}) - \langle O_N \rangle$ representing the fluctuations of the intra-unit-cell nematicity. By eye, nearly all the topological defects appear located in white regions of vanishing $\delta O_N(\vec{r}) = 0$. This can be quantified by plotting the distribution of distances of topological defects from the nearest zero of $\delta O_N(\vec{r}) = 0$, thereby showing that they are far smaller than expected if the topological defects were uncorrelated with $\delta O_N(\vec{r})$ (Fig.3e inset). These data provide empirical evidence for a coupling between the smectic topological defects and the fluctuations of the intra-unit-cell nematicity at $E \sim \Delta_1$.

When $Z(\vec{r},E)$ images of the intra-unit-cell electronic structure in underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ are analyzed using two independent techniques, compelling evidence for intra-unit-cell (or $\vec{Q}=0$) electronic symmetry breaking is detected specifically of the states at the $E \sim \Delta_1$ pseudogap energy. Moreover, this intra-unit-cell symmetry breaking coexists with finite $\vec{Q} = \hat{S}_x,\hat{S}_y$ smectic electronic modulations, and the coupling between these states are through the $2\pi$ topological defects creating spatial fluctuation of the nematicity.

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