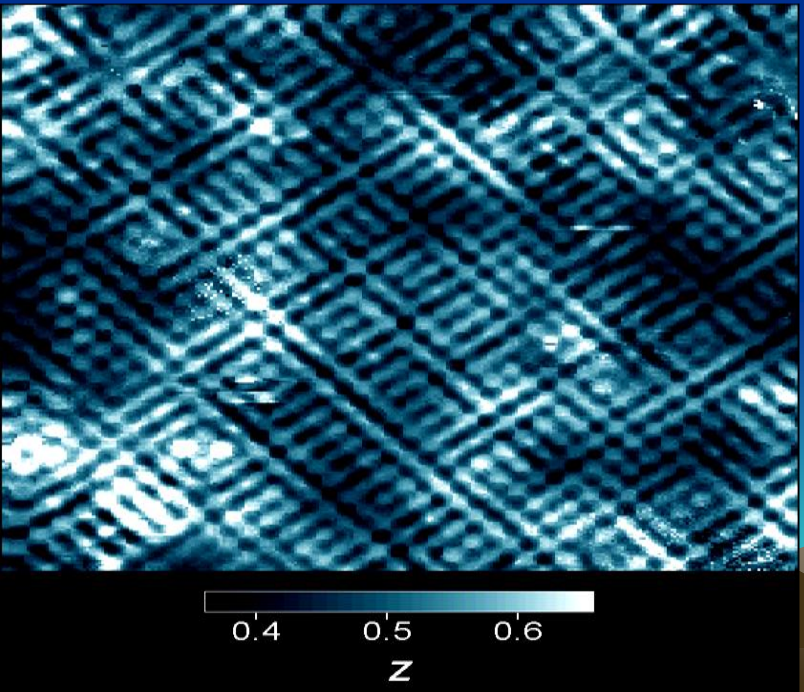
Atomic Scale Rotational Symmetry Breaking in Sodium Doped Cuprates

Fu-Chun Zhang

The Univ. of Hong Kong



collaborators

Yan Chen (HKU)

T. M. Rice (ETH)

Outline

1. Introduction

   Recent STM on Ca(2-x)Na(x)CuO(2)Cl(2) by Kohsaka et al. –Davis group

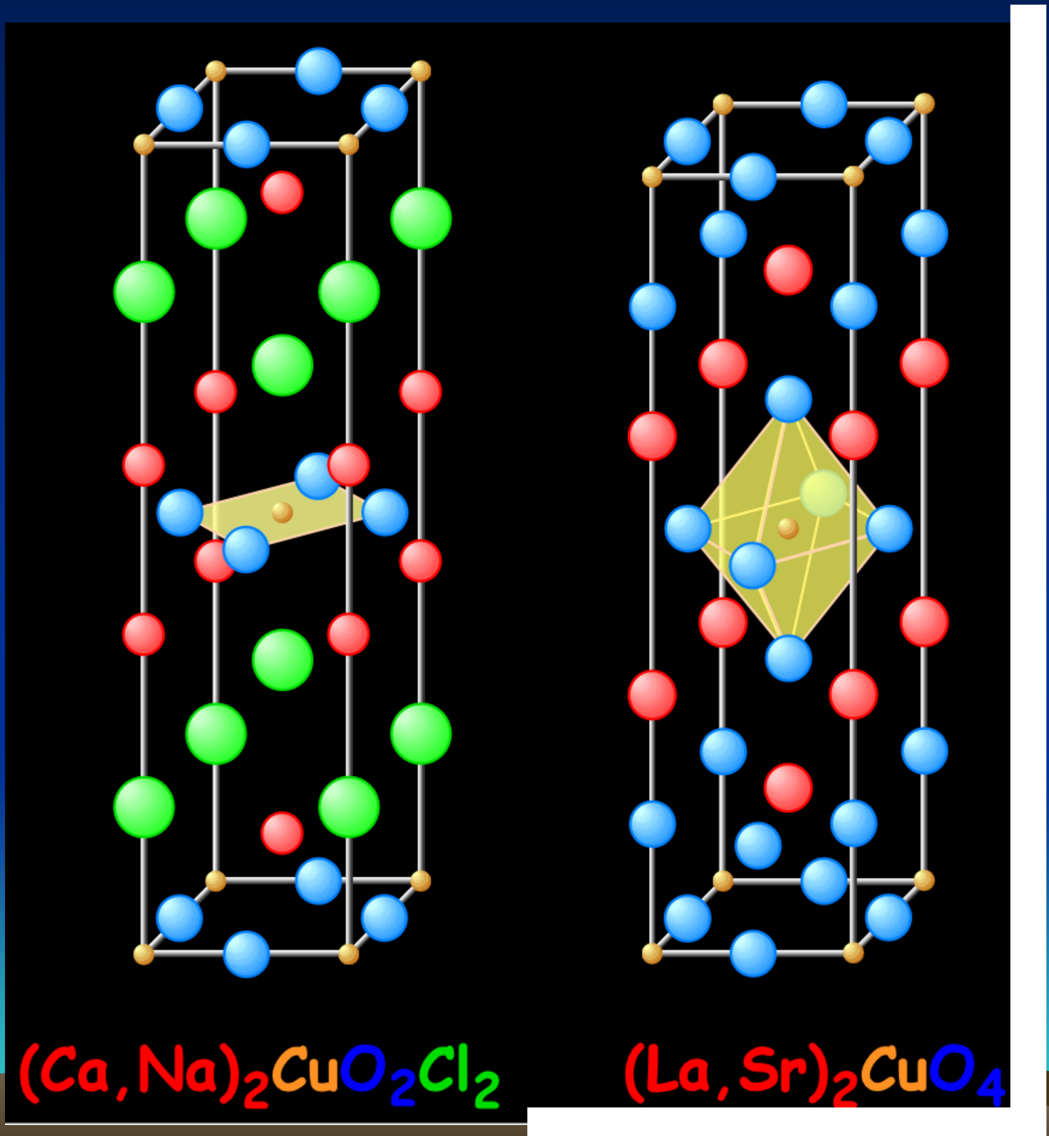
2. Theory

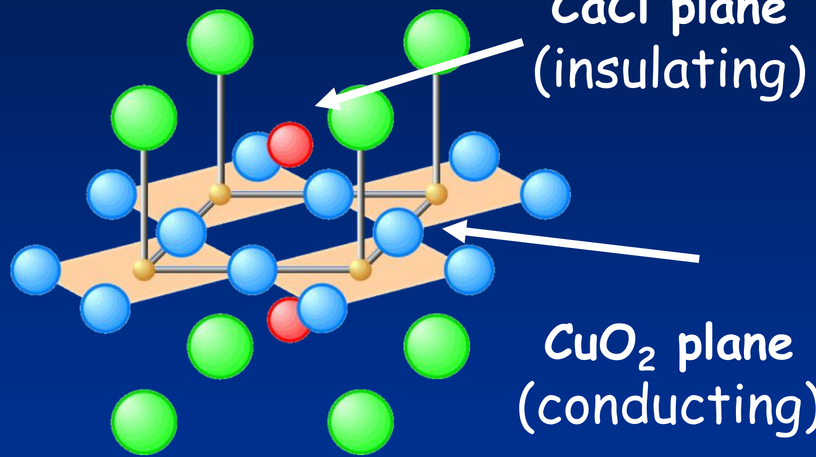
   Doubly degenerate ground states

   Anisotropy of conductance

3. Summary

Crystal structure of $Ca_{2-x}Na_xCuO_2Cl_2$

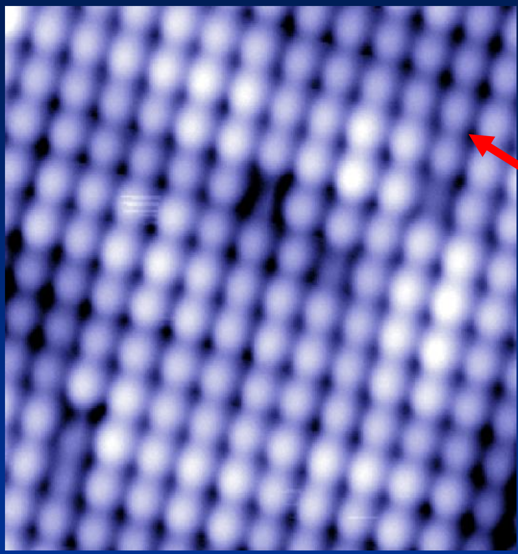




- STM measures local differential conductance dI/dV

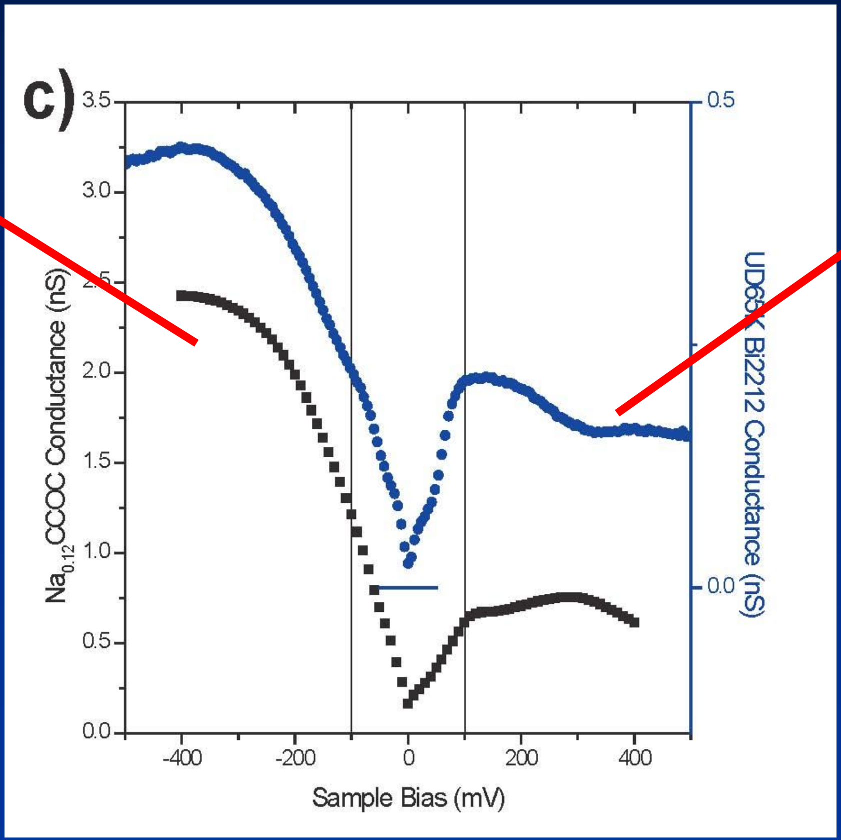
~ local electron density of states n(r, E)

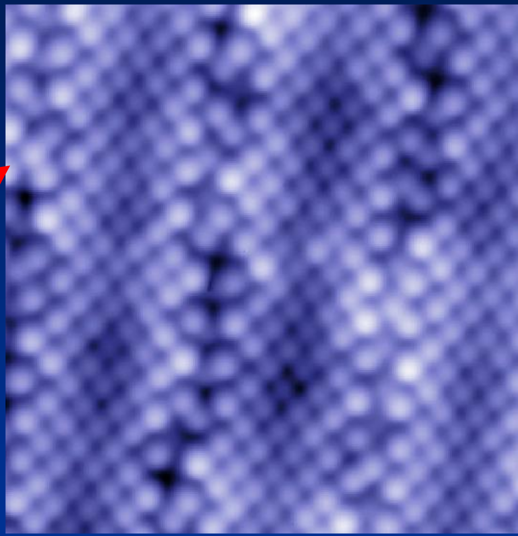
Asymmetry in Tunneling



$Ca_{1.9}Na_{0.1}CuO_2Cl_2$

x~0.1±0.01





$Bi_2Sr_2CaCu_2O_{8+x}$

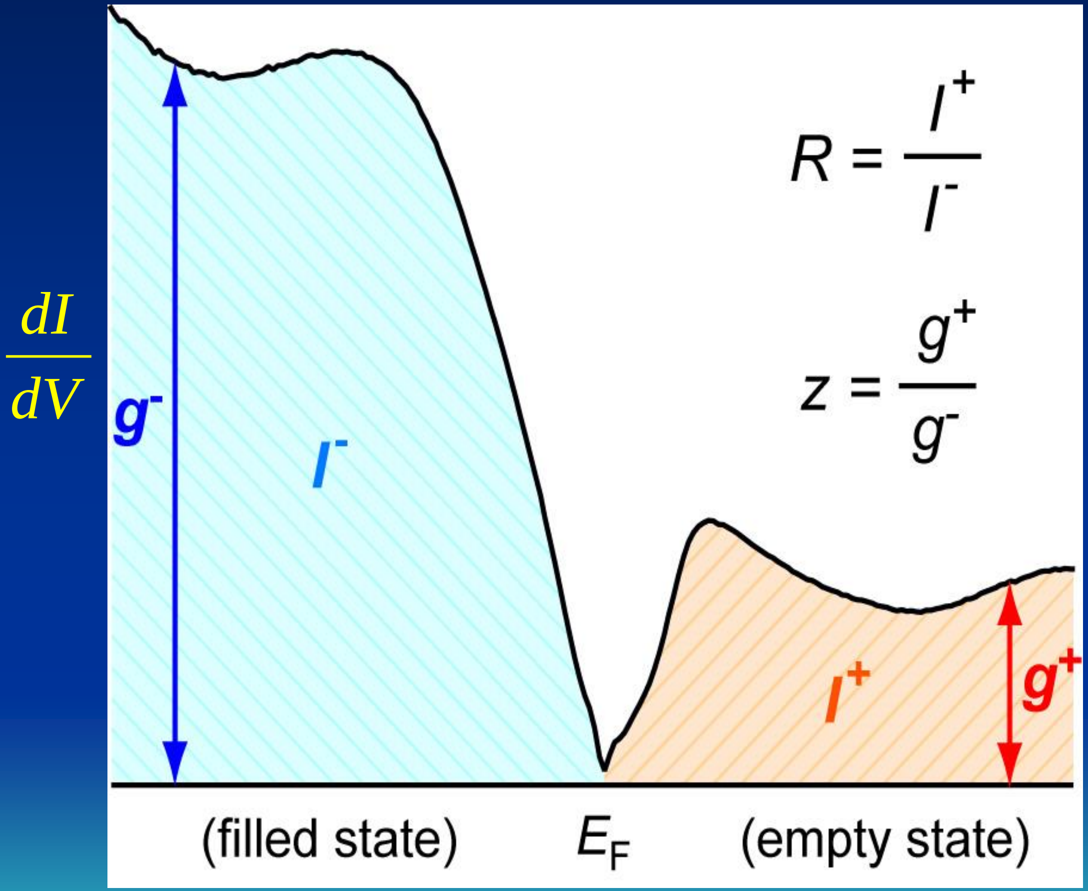
x~0.1±0.01

Asymmetric conductance spectrum is characteristic of doped cuprates.

Left side: injection of a hole; **Right side: injection of an electron.**

Mott physics: each Cu-site only allow 1 electron, spin-up or -down, so that injection of an electron is much more difficulty than injection of a hole

A new STM hole-density imaging techniques: Z map and R map (Davis group)



$$Z = \frac{g^{+}(V)}{g^{-}(V)} \sim \frac{2p}{(1-p)}$$

Anderson & Ong, (2004).

$$R = \frac{\int_{0}^{eV} dE\, N(E)}{\int_{-eV}^{0} dE N(E)} \approx \frac{2p}{(1-p)}$$

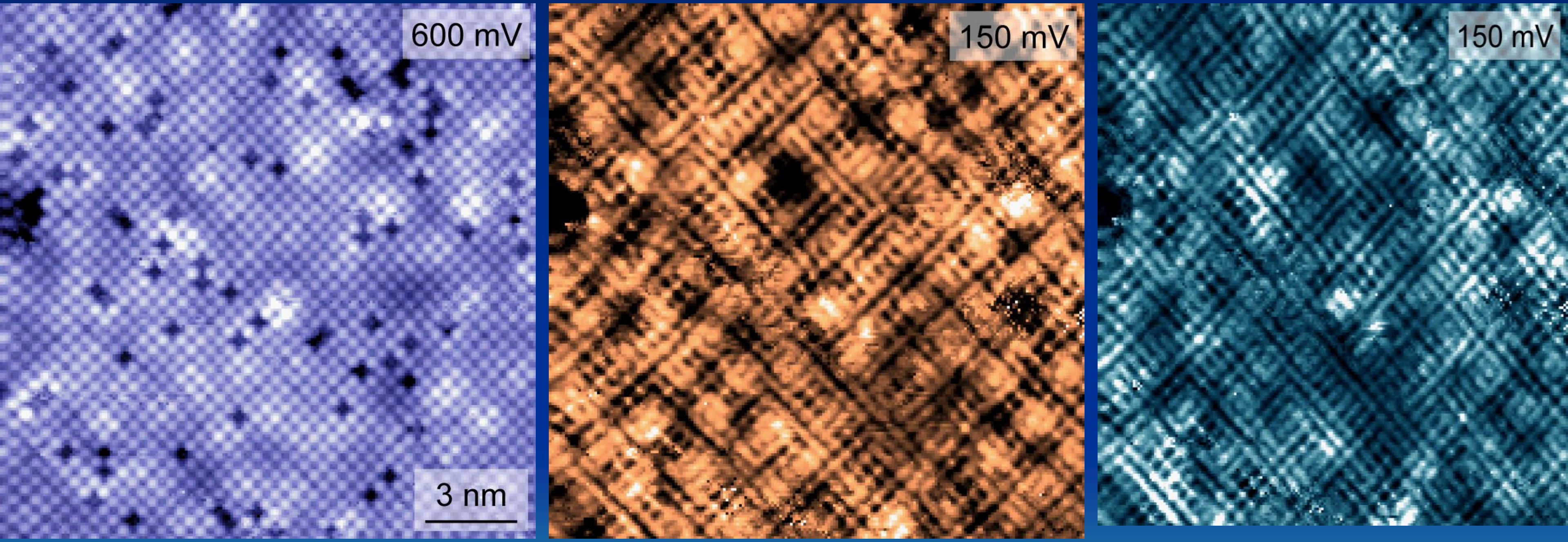
Randeria, Sensarma, Trivedi, & FC Zhang, (2004), PRL 95 (2005).

p: hole density

Measures local hole density independent of strength of troublesome tunneling matrix

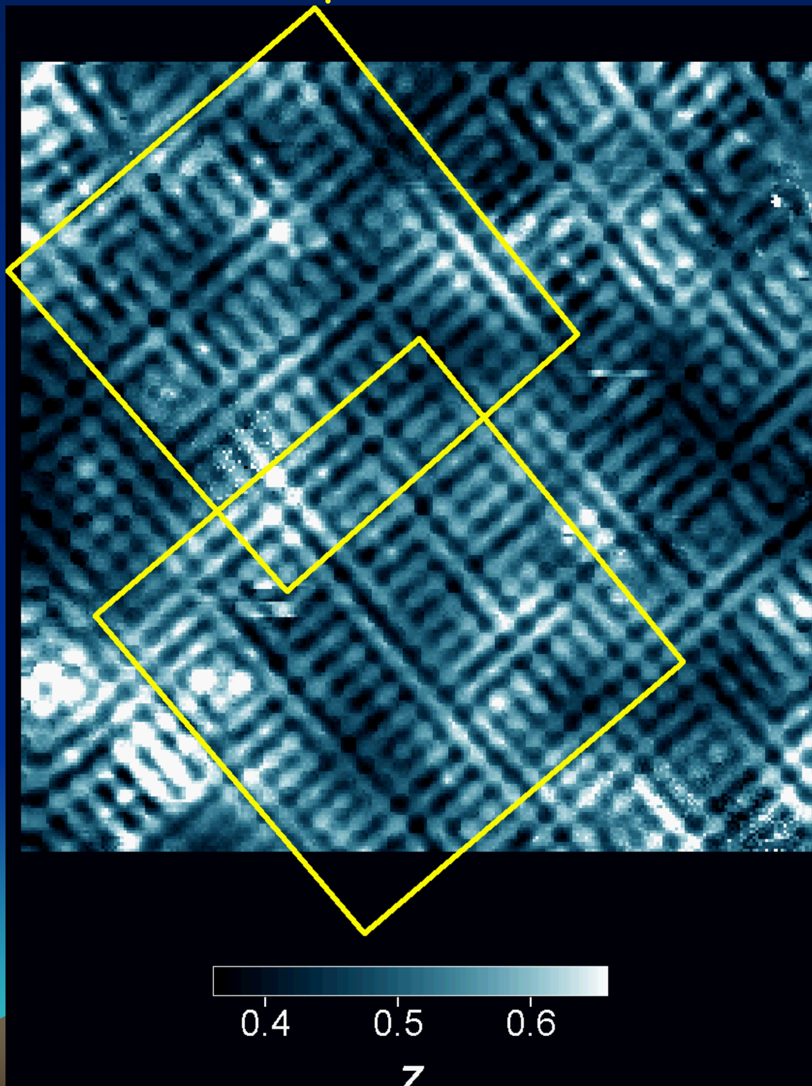
Atomic scale rotational and translational symmetry breaking

topo R map Z map

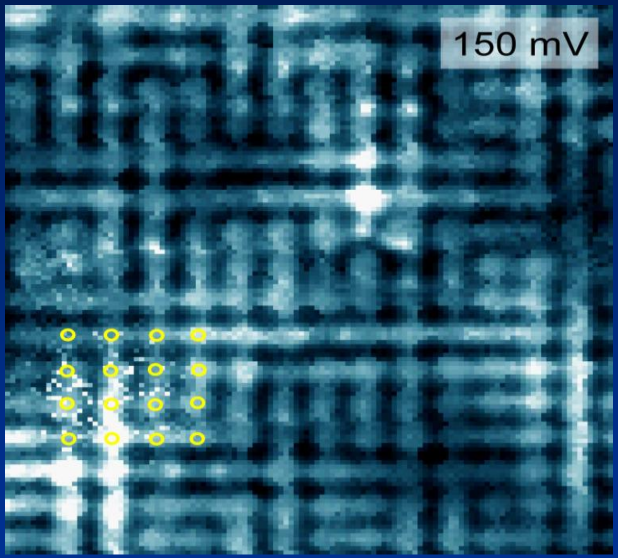


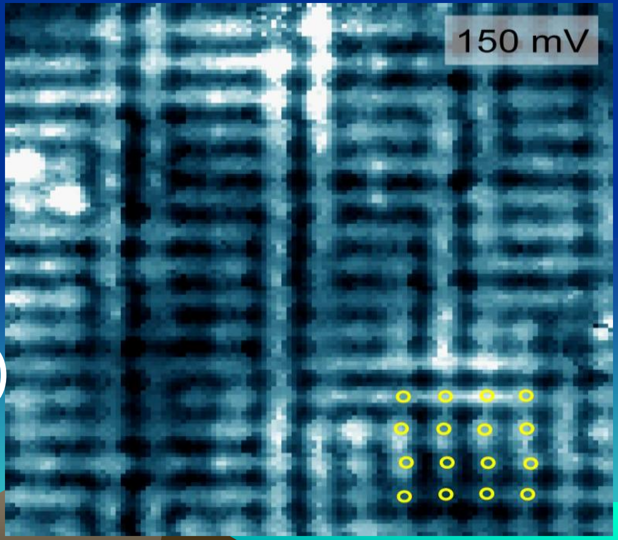
Atomic scale rotational and translational symmetry breaking

z map (150 mV)



$Z=2p/(1-p)$



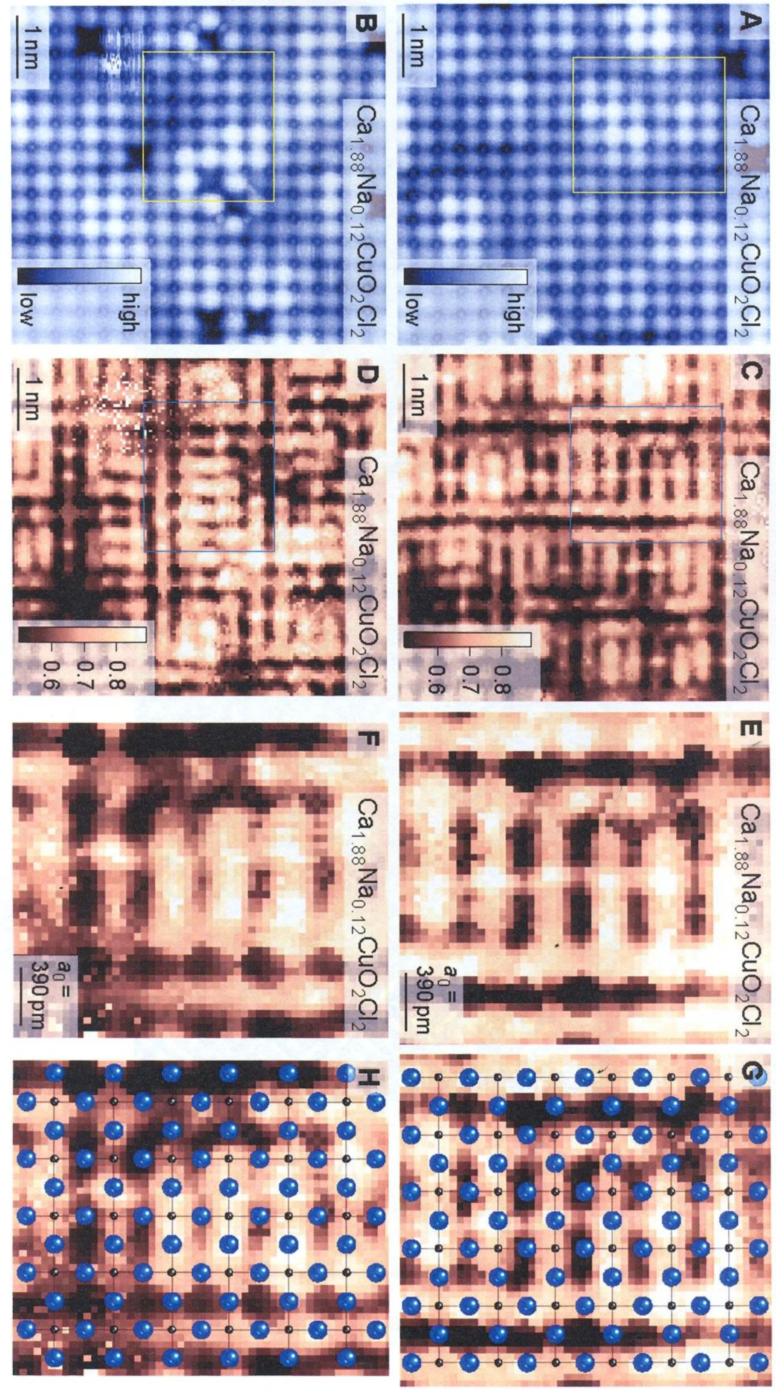


Y. Kohsaka *et al , prepared*

Data from Davis' group

Topographic images (600 meV)

R-map (150 meV) , Break translational & Rotational symmetry



Contrast in R most at O-sites (blue ones)

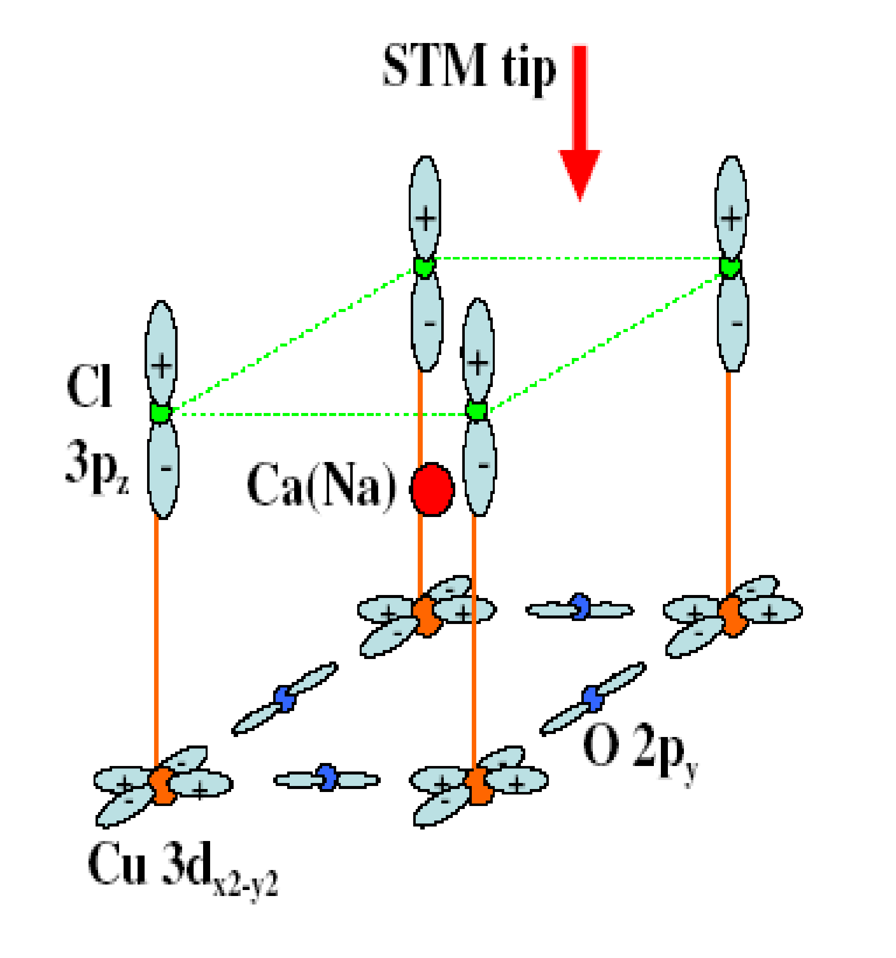
Theoretical issues

- The attractive potential generated by Na-acceptor does not break the local square symmetry, why the rotational symmetry is broken in the STM experiments?
- Why is strong asymmetry respected with STM on the O-sites?

2. Theory

1) Theory of STM
2) Reflection symmetry of square lattice
3) Symmetry of the ground state of t-J cluster
4) Anisotropy of STM spectra

Theory of the STM: formalsim (1)



No matrix element between Cl and Cu directly below.

$\Psi_0^{1h}, p_{Cl,i,\sigma}$ **single hole w.f. of the Cu-O plane, and Cl-hole**

$$
\begin{aligned}
p^{\dagger}_{Cl,\vec{i},\sigma}|\Psi_0^{1h}\rangle &\propto \sum_{\vec{\tau}} \langle \vec{i}, Cl|\vec{i}+\vec{\tau}, Cu\rangle c^{\dagger}_{\vec{i}+\vec{\tau},\sigma}|\Psi_0^{1h}\rangle \\
&\propto \sum_{\vec{\tau}} (-1)^{M_{\vec{\tau}}} c^{\dagger}_{\vec{i}+\vec{\tau},\sigma}|\Psi_0^{1h}\rangle
\end{aligned}
$$

relative phase

Assuming square lattice is four-fold rotational invariant

superposition in hole-states centered on the four n.n. Cu-site

Theory of the STM, formalism (II)

When the tip is above the two neighboring Cl sites, we have

$$a^\dagger_{\vec{r},\sigma}|\Psi_0^{1h}\rangle = [\langle\vec{r}|\vec{i},Cl\rangle p^\dagger_{Cl,\vec{i},\sigma} + \langle\vec{r}|\vec{i}+\vec{\tau}',Cl\rangle p^\dagger_{Cl,\vec{i}+\vec{\tau}',\sigma}]|\Psi_0^{1h}\rangle$$

The differential conductance is (Tersoff and Hamann, 85')

$$\frac{dI(\vec{r})}{dV} \propto \sum_{\sigma,m} |\langle m|a^\dagger_{\vec{r},\sigma}|\Psi_0^{1h}\rangle|^2 \delta_{E_m - E_0^{1h},\omega}$$

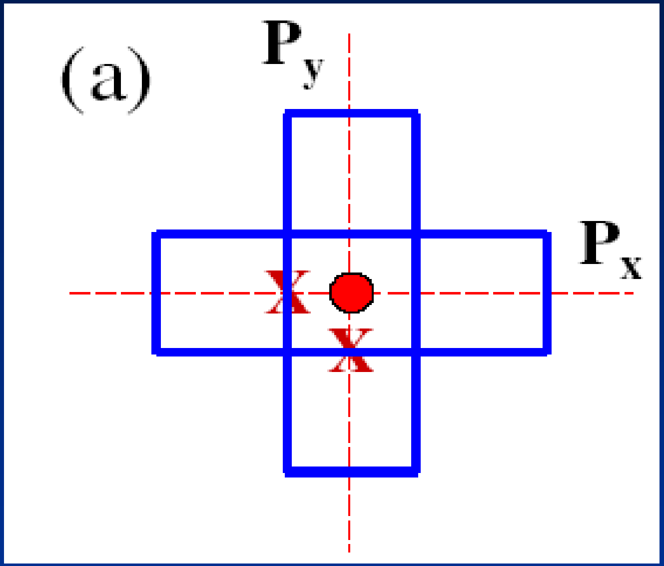
omega=eV

The integrated current up to a positive voltage is, **As tip scans from i to i+tau'**

$$I(\vec{r},\omega) = A\sum_{\sigma,m} |\langle m|\sum_{\vec{\tau}}(-1)^{M_{\vec{\tau}}}[\langle\vec{r}|\vec{i},Cl\rangle c^\dagger_{\vec{i}+\vec{\tau},\sigma} + \langle\vec{r}|\vec{i}+\vec{\tau}',Cl\rangle c^\dagger_{\vec{i}+\vec{\tau}'+\vec{\tau},\sigma}|\Psi_0^{1h}\rangle|^2\Theta(\omega - E_m + E_0^{1h})$$

The tunneling conductance will be sensitive to the relative phase to inject electrons on n.n. Cu sites. We need to examine carefully the symmetry of the ground state wavefunction.

Theory of the STM: tunneling above O-site



The red cross denotes the tip position above the oxygen atoms along the x- and y-axes.

So the integrated differential conductance at the position of two crosses can be expressed as

$$I^{x(y)}(\omega) = \sum_{\sigma} I_{\sigma}^{x(y)}(\omega),$$

$$I_{\sigma}^{x(y)}(\omega) = A_0 \sum_{m} |\langle m| \sum_{\vec{\tau}} (-1)^{M_{\vec{\tau}}} (c^{\dagger}_{\vec{i}+\vec{\tau},\sigma} + c^{\dagger}_{\vec{i}+\hat{x}(\hat{y})+\vec{\tau},\sigma}) |\Psi_0^{1h}\rangle|^2 \Theta(\omega - E_m + E_0^{1h}),$$

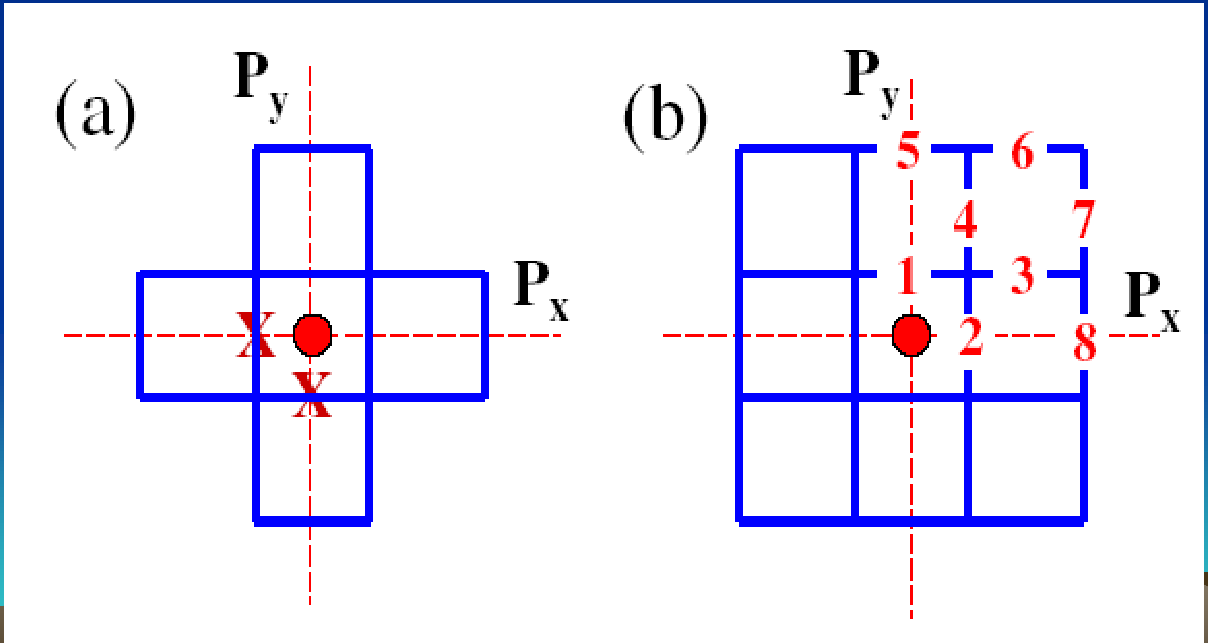
the ratio of the conductance at the two positions.

$$\eta(\omega) = I^x(\omega)/I^y(\omega)$$

Reflection symmetry

In 2D square lattice, focus on the reflection symmetries with respect to x- and y-axes. Classify states according to the quantum numbers of Px and Py.

Px (Py) $\psi_0 = \psi_0$ even (+), Px (Py) $\psi_0 = -\psi_0$ odd (-)



Three types of phases,

(I) Px, Py (+,+) Non-degenerate

(II) (+, -) and (-,+) doubly degenerate

(III) (-,-) non- degenerate

Ground State of one hole in t-t'-J cluster

t-t'-J cluster with on site impurity potential

$$\mathcal{H} = -\sum_{i,\sigma} \epsilon_i c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle i,j\rangle\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{h.c.}) - t' \sum_{\langle\langle i,j\rangle\rangle\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{h.c.}) + J \sum_{\langle i,j\rangle} \boldsymbol{S_i} \cdot \boldsymbol{S_j}.$$

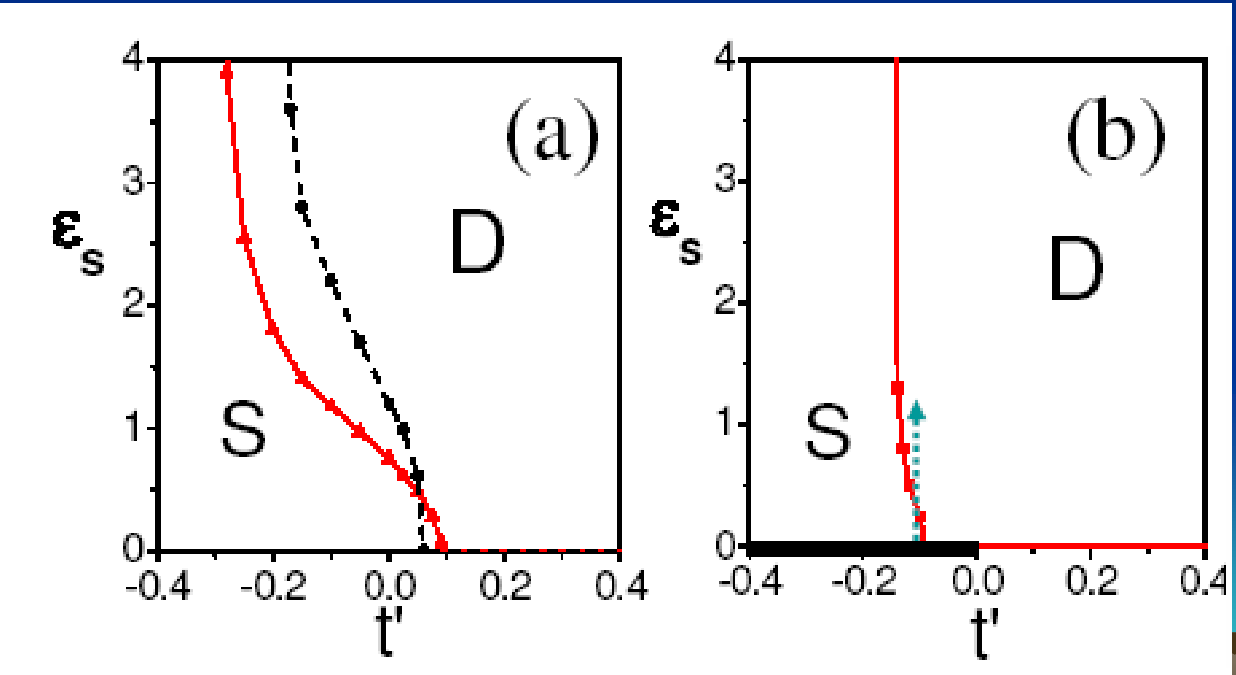
Previous studies:

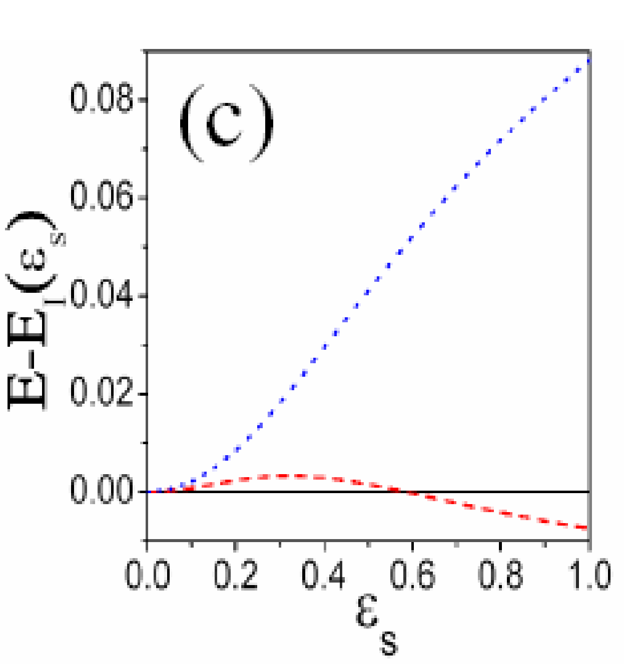
1) **ε_i=0, 4x4 for periodic boundary condition, 4-fold symmetry for t'<0 and 2-fold symmetry for t'>0.**
   Gagliano et al, 1992.
2) **t'=0, doubly degenerate states in certain parameter regime.**
   Szczepanski et al., 1989, Rabe & Bhatt 1991, Gooding 1991.

Ground States of t-t’-J cluster

(a) And (b): ground states from cluster cal. (t=1, J=0.3)
For sodium doped cuprates, t’~-0.1.
(c): energy level as a function of ε_s . Large impurity strength may prefer doubly degenerate state

S: singly degenerate state; D: doubly degenerate state



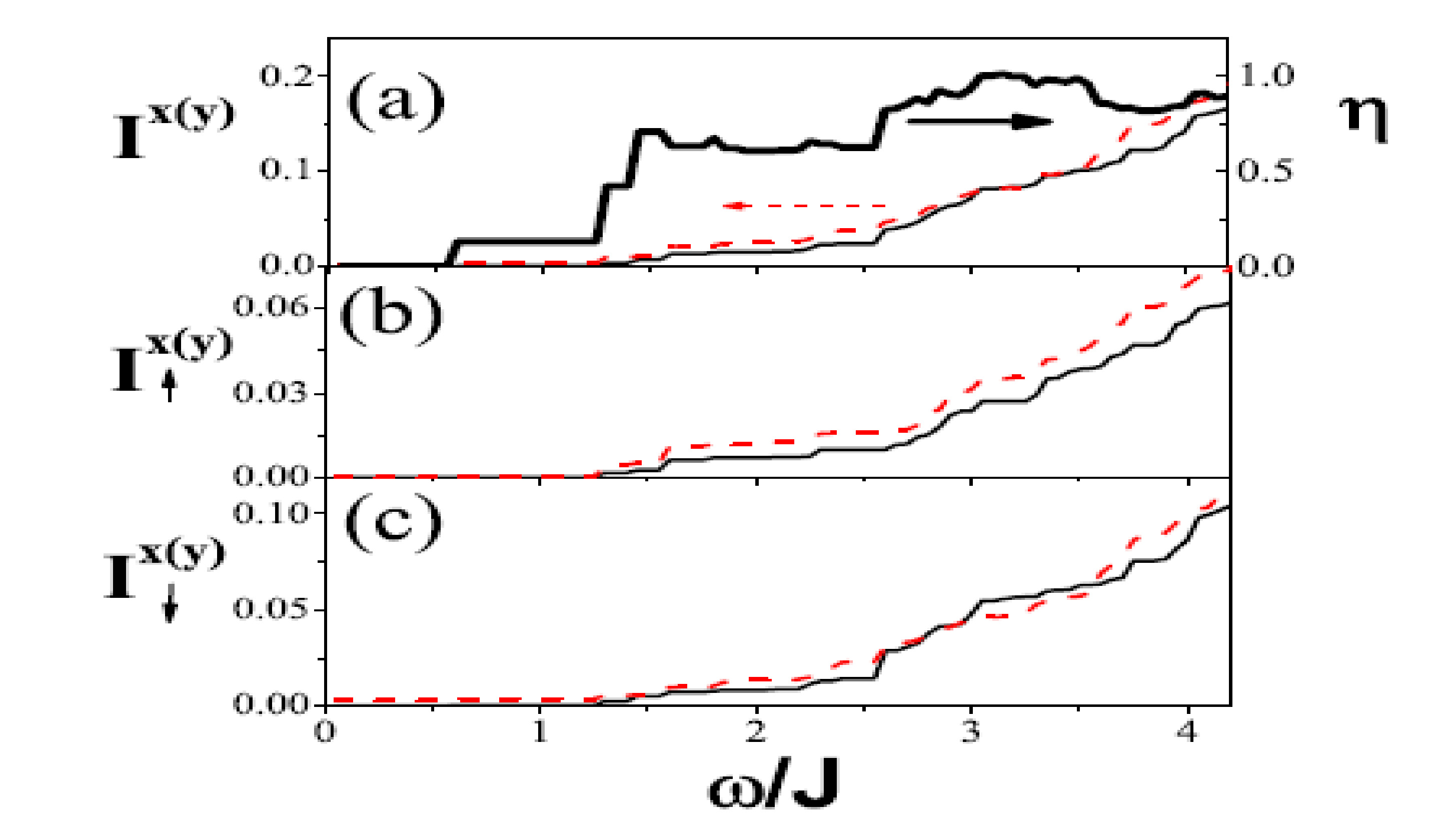


open boundary

Periodic 16 sites

t’=-0.12, red: 2-fold

STM spectra of 2-fold degenerate ground state of single hole in 12-site cluster



Strong asymmetry at lower energy while asymmetry becomes much weaker at higher energy. Asymmetry is also strongly spin-dependent. A spin-resolved STM may detect such asymmetry more effectively.

STM spectra of 4-site cluster with 1 hole

The ground state is doubly degenerate, with

$$E_g = -J/2 - \sqrt{3t^2 + (t' + J/2)^2},$$

and $$tan\gamma = \sqrt{3}t/(J + t' + E_g)$$

We find that $I^x_\uparrow(\omega) = \frac{4}{3}\cos^2\gamma\Theta(\omega - J),\ I^x_\downarrow(\omega) = \frac{2}{3}\cos^2\gamma\Theta(\omega - J),$

and $I^y_\uparrow(\omega) = 0$ and $I^y_\downarrow(\omega) = \cos^2\gamma\Theta(\omega) + \sin^2\gamma\Theta(\omega - 2J).$

Summing over spins,

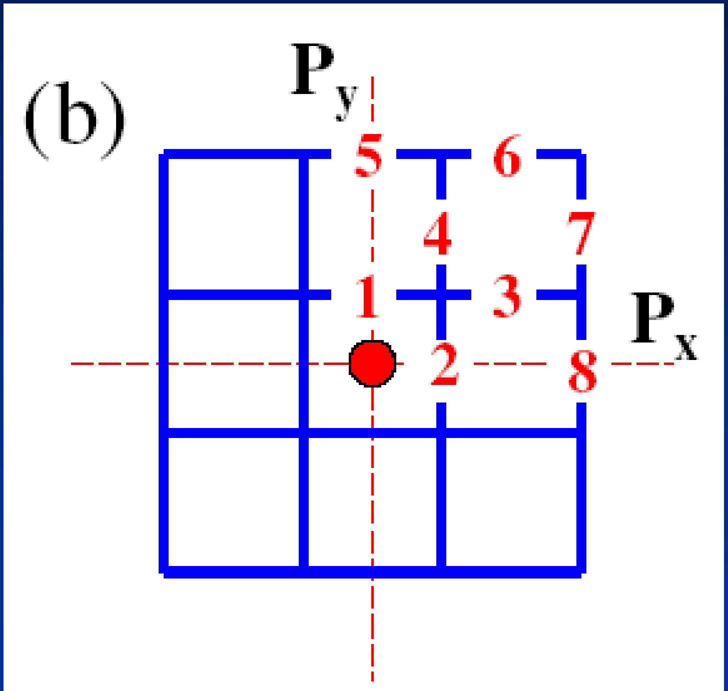
$$I^x(\omega) = I^x_\uparrow + I^x_\downarrow = 2\cos^2\gamma\Theta(\omega - J)$$

$$I^y(\omega) = \cos^2\gamma\Theta(\omega) + \sin^2\gamma\Theta(\omega - 2J).$$

So the ratio $\eta(\omega)$ >>1 for omega (0,J), $\eta(\omega)$=1/2 for (J,2J) while

$\eta(\omega) = 2\cos^2\gamma$ for very high energy. (For t'/t=-0.1, $\eta(\omega)$~0.97.)

Spatially dependent correlations



Hopping integral and spin-spin correlation function for various bonds in a 16-site cluster with PBC.

bond index	1	2	3	4	5	6	7	8
$\langle C_i^\dagger C_j \rangle$	0.342	0.328	0.122	0.129	0.020	0.014	0.012	0.016
$-\langle S_i S_j \rangle$	0.167	0.074	0.161	0.167	0.329	0.336	0.347	0.334

The strong variations of parameters around the impurity may lead to the formation of local lattice distortion which may induce further rotational asymmetry.

Summary

- **STM shows local square rotational symmetry breaking**
- A simple theory:

  1. Double degeneracy of the ground state for small clusters

  2. Breaking of rotational symmetry may lead to anisotropic conductance pattern as the tip scans above O-site along the x – and y-axes

  3. The strong anisotropy is at low voltage cut-off while the anisotropy becomes weaker at higher voltage cut-off