Hoffman Lab Microscopes

V E C R I



High-T_c Superconductivity



Picoscale atomic distortion



Nature Materials 11, 585 (2012)

Single oxygen atoms



Science 343, 390 (2014)

d-wave charge ordering



arxiv:1402.5415



Fermi surface transition



Science 344, 608 (2014)





V E 🎽 R



V E 🎽 R





WKB says that the tunneling probability through a barrier will be $|M|^2 = e^{-2\gamma}$ where:

$$\gamma = \int_0^s \sqrt{\frac{2m\varphi}{\hbar^2}} dx = \frac{s}{\hbar} \sqrt{2m\varphi} \longrightarrow I \approx \frac{4\pi e}{\hbar} e^{-\frac{1}{s}\sqrt{\frac{8m\varphi}{\hbar^2}}} \rho_t(0) \int_{-eV}^0 dx$$

s = tip-sample distance φ = tip-sample work function

Details: Tersoff & Hamman, PRL 50, 1988 (1983) & PRB 31, 805 (1985)

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 $\rho_s(\varepsilon)d\varepsilon$

STM: setup condition





 \rightarrow Define:

Z-maps









P. W. Anderson, N. P. Ong, *J. Phys. Chem. Solids* 67, 1 (2006).

Experiment:

$$Z(\vec{r}, V) \equiv \frac{\frac{\mathrm{d}I}{\mathrm{d}V}(\vec{r}, z, +V)}{\frac{\mathrm{d}I}{\mathrm{d}V}(\vec{r}, z, -V)}$$

R-maps

Theory:

Randeria, *PRL* **95**, 137001 (2005).

VE RI TAS

Experiment:

$$R(\vec{r}, V) \equiv \frac{I(\vec{r}, z, +V)}{I(\vec{r}, z, -V)}$$

Z vs. R maps

Z vs. R maps			VE RI TAS
	Ζ	R	HARVARD
Theory:	$\frac{\overline{N}(E = +eV)}{\overline{N}(E = -eV)} \approx \frac{2n}{1+n}$ Anderson, <i>JPCM</i> (2006)	$\frac{\int_{0}^{\Omega_{c}} N(\vec{r}, E) \mathrm{d}E}{\int_{-\infty}^{0} N(\vec{r}, E) \mathrm{d}E} = \frac{2n(\vec{r})}{1 - n(\vec{r})}$ Randeria, <i>PRL</i> (2005)	
Experiment:	$Z(\vec{r}, V) \equiv \frac{\frac{\mathrm{d}I}{\mathrm{d}V}(\vec{r}, z, +V)}{\frac{\mathrm{d}I}{\mathrm{d}V}(\vec{r}, z, -V)}$	$\frac{I(\vec{r}, z, +V)}{I(\vec{r}, z, -V)}$	
Advantages:	Divides out the	setup condition artifact!	
	Maintain energy resolution	Integrate over all energies, integrates a small signal, catches a signal at unknown er	nergy.
Disadvantage	s: <u>Assumes particle-hol</u>	e symmetry of the signal of interest!	
		Lose energy resolution. What cutoff to use? Theory: $\Omega_c \sim 1 \text{ eV}$; Expt: V = 15	50 mV
In practice:	QPI	static checkerboards	

Types of STM Measurements







STM: pros & cons



Advantages

- Filled and empty states
- sub-meV energy resolution
- B-field dependence
- Atomic spatial resolution
- k-information w/ nanoscale resolution (via QPI)

Challenges

- Surface sensitivity
- polarity, termination, reconstruction
- vibration sensitivity

- 1960: gap measurement (Pb)
- 1965: boson energies & coupling (Pb)
- 1985: charge density wave (TaSe₂)
- 1989: vortex lattice (NbSe₂)
- 1997: single atom impurities (Nb)
- 2002: quasiparticle interference
 - → band structure & gap symmetry (BSCCO)
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1960: Tunneling measurements of Δ



VOLUME 5, NUMBER 4

PHYSICAL REVIEW LETTERS

August 15, 1960

ENERGY GAP IN SUPERCONDUCTORS MEASURED BY ELECTRON TUNNELING

Ivar Giaever General Electric Research Laboratory, Schenectady, New York (Received July 5, 1960)



Giaever, PRL 5, 174 (1960)

Structure of $Bi_2Sr_2CaCu_2O_{8+\delta}$





Δ inhomogeneity in BSCCO





Suggests the existence of a local "hidden" variable we could use to control Δ ? (and raise Tc?)

100

Δ inhomogeneity in BSCCO

VE RI TAS



McElroy, PRL 94, 197005 (2005)

Inhomogeneity of $T(\Delta \text{ closure})$ in BSCCO



Tc=65K (overdoped)





Gomes, Nature 447, 569 (2007)

Are oxygen dopants causing inhomogeneity?

VE RI TAS FERVARD

Conclusions about interstitial oxygen:

(1) Observed at -0.96 V in dl/dV

(2) "Strong correlations" exist between these oxygen dopants and "the gap"

(3) These oxygen dopants are primarily positioned in the minima of the "QPI"

dI/dV at -1V



gapmap

20 meV _____ 70 meV

dI/dV at -24 mV



McElroy, Science 309, 1048 (2005)

Puzzle: local trend opposes global trend





Zhou prediction: type-A oxygen

B-site disorder: (e.g. Pb^{2+} on Bi^{3+} site or Y^{3+} on Ca^{2+} site) does not couple to CuO_2



Eisaki, PRB 69, 064512 (2004)

interstitial O in BiO plane weakly couples to CuO_2 provides charge carriers but little local effect \rightarrow "type-B oxygen"



seen at -0.96V McElroy, Science 309, 1048 (2005)



A-site disorder: (Bi³⁺ on Sr²⁺ site) strongly couples to apical O



claim: seen at +1.8V Kinoda, PRB 67, 224509 (2003)

interstitial O in SrO plane strongly couples to CuO_2 provides charge carriers and disorder

→ "type-A oxygen"



expected << -1V

Mapping additional dopants (T_c =55K)





B Oxygen +1V, unknown ???



Zelkjovic + JEH, Science (2012)

Spectral signatures (T_c=82K)



Zelkjovic + JEH, Science (2012)

VE RI

Tc = 55K





29 x 29 nm²

Tc = 55K



 \bigcirc 8 0 \mathbf{O} ()

• O, type-A

expect $O_A(r) \times \Delta(r) < 0$ (causality)

 \rightarrow NOT OBSERVED



29 x 29 nm²

Tc = 55K





apical O vacancy



29 x 29 nm²

Resolved! local vs. global dependence



Zelkjovic + JEH, Science (2012)

V E 🞽 R I

Part I: Conclusions



- Doubled the energy range for local spectroscopy on BSCCO
- Found all oxygen dopants: type-A & B oxygen, apical O vacancies
- apical O vacancies
 - strongly enhance the gap energy
- * type-A oxygens
 - attracted to apical O vacancies in UD
 - control local charge in OPT
- type-B oxygens
 - weakly correlate, secondary effect

Next steps:

- control dopants to raise T_c ??
- fit to find effective charge & radius of dopants
- understand how dopants affect CDW

Theory: Goren, Altman, PRB 84, 094508 (2011)

apical O vacancy



doping (p_1)

Superconductivity Tunneling Milestones

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ARPES: first evidence of gap anisotropy

VOLUME 70, NUMBER 10

PHYSICAL REVIEW LETTERS



8 MARCH 1993

Anomalously Large Gap Anisotropy in the a-b Plane of Bi₂Sr₂CaCu₂O_{8+s}

Z.-X. Shen,^{(1),(2)} D. S. Dessau,^{(1),(2)} B. O. Wells,^{(1),(2),(a)} D. M. King,⁽²⁾ W. E. Spicer,⁽²⁾ A. J. Arko,⁽³⁾ D. Marshall,⁽²⁾ L. W. Lombardo,⁽¹⁾ A. Kapitulnik,⁽¹⁾ P. Dickinson,⁽¹⁾ S. Doniach,⁽¹⁾ J. DiCarlo,^{(1),(2)} A. G. Loeser,^{(1),(2)} and C. H. Park^{(1),(2)}



Questions

VE RI TAS FARVARD

1. What is the pairing symmetry of a superconductor?



2. Where on the Fermi surface does the pairing occur?



How can disorder help us?





H₂O

ME (experimentalist)



perturbation

interference patterns

Bi₂Sr₂CaCu₂O_{8+d}





First QPI: metals, real space





Crommie, Lutz & Eigler, Nature <u>363</u>, 524 (1993)





Peterson, Hofmann, Plummer & Besenbacher, J. Electron Spectroscopy 109, 97 (2000)

2-dim band structure: topographic map for e





Contours of

Constant Energy

Standard Routes

k,

The real theory...

Density of states:

1

$$n(\mathbf{q}, \omega) = n_0(\mathbf{q}, \omega) - \frac{1}{2\pi i} [A_{11}(\mathbf{q}, \omega) + A_{22}(\mathbf{q}, -\omega) - A_{11}^*(-\mathbf{q}, \omega) - A_{22}^*(-\mathbf{q}, -\omega)]$$

$$A(\mathbf{q}, \omega) = \int \frac{d^2k}{(2\pi)^2} G_0(\mathbf{k} + \mathbf{q}, \omega) T(\mathbf{k} + \mathbf{q}, \mathbf{k}; \omega) G_0(\mathbf{k}, \omega)$$

$$scattering$$
Greens functions
$$\rightarrow \text{There will be cross terms.}$$

$$Wang \& Lee, PRB 67, 020511 (2003)$$

But empirically, simple real model is a good approximation to the data:

$$\mathbf{P}(\varepsilon, \mathbf{\vec{q}}) \propto \left| \mathbf{V}(\mathbf{\vec{q}}) \right|^2 \mathbf{n}_i(\varepsilon_i, \mathbf{\vec{k}}_i) \mathbf{n}_f(\varepsilon_f, \mathbf{\vec{k}}_f)$$

McElroy, PRL 96, 067005 (2006)

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ARPES: Normal State Fermi Surface & Band Structure



ARPES: Superconducting anisotropic gap $\Delta(k)$



Ding et al., PRLB 54, 9678 (1996)



Shen *et al*, PRL **70** 1553 (1993) Ding *et al*, PRB **54** 9678 (1996) Mesot *et al*, PRL **83** 840 (1999)

0 meV CCE: the Fermi points











Octet of regions at ends of 'bananas' have largest |dk|/dE



Density of States

$$n(E) = \oint_{E(k)=E} \frac{1}{\left| \nabla_{k} E(\vec{k}) \right|} dk$$

The octet of k-space locations at the tips of the 'bananas' provide maximum contribution to $n_{i,f}(E)$ and thus dominate elastic scattering processes.



k-space:

- unperturbed eigenstates
- not directly accessible to STM
- measured by ARPES



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- measured by ARPES

q-space:

• Scattering \rightarrow standing waves $q = 2\pi/\lambda$

 $\rightarrow \vec{q}_1$

(π,π**)**

(π,**0**)



k-space:

- unperturbed eigenstates
- not directly accessible to STM
- measured by ARPES

q-space:

• Scattering \rightarrow standing waves $q = 2\pi/\lambda$

(π,π)

(π,0**)**

 \vec{q}_2



k-space:

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- measured by ARPES

q-space:

• Scattering \rightarrow standing waves $q = 2\pi/\lambda$

(π,π)

(π,**0**)

 \vec{q}_3

 \vec{q}_2



k-space:

- unperturbed eigenstates
- not directly accessible to STM
- measured by ARPES

q-space:

• Scattering \rightarrow standing waves $q = 2\pi/\lambda$

 \vec{q}_4

(π,π)

(π,**0)**

 \vec{q}_3

 \vec{q}_2



k-space:

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- Scattering \rightarrow standing waves $q = 2\pi/\lambda$
- Measure q from FT of LDOS image





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Expected structure of FFT of LDOS(r,E) (for a fixed E)



Dispersion:

how does each $\vec{q_i}$ vary with E?

For example, look at the dispersion of: $\vec{q_1} \mid \mid (\pm \pi, 0)$ or $(0, \pm \pi)$















(π,π)

(π,0)











For example, look at the dispersion of: $\overline{q_7} \mid \mid (\pm \pi, \pm \pi)$

























Expected energy dependence of 5 independent qi's





$Bi_2Sr_2CaCu_2O_{8+d}$ Data

topograph

A. AN THE STAR AR

545 Å

Bi-2212 $T_c=76 \text{ K}$ $\Delta \sim 51 \text{meV}$



energy (meV) Imaging quasiparticle wavefunctions $g(\vec{r}, \vec{E})$ $g(\vec{q}, \vec{E}) = \sqrt{P(\vec{q}, \vec{E})}$ $(0, 2\pi)$ FFT

545 Å

Bi-2212 T_c=76 K ∆~51meV



(2π,0)



Bi-2212 T_c=76 K ∆~51meV








 $T_c=76 \text{ K}$ $\Delta \sim 51 \text{meV}$

































Measuring the dispersion of the $q_i(E)$



McElroy, Nature, 222, 592 (2003)

ARPES & STM: Fermi surface comparison



McElroy, Nature, 222, 592 (2003)

QPI persists to $> 1.5*T_c$



Motivation: QPI is p-h symmetric. Claim: no state other than superconductivity is p-h symmetric. Therefore, QPI is marker for SC.

V E 🎽 R



Caveat: these are Z maps \rightarrow they assume p-h symmetry

Lee, ... Davis, Science 325, 1099 (2009)

nesting wavelength vs. local and global Δ



- hole pocket expands with doping
 - nesting wavevector decreases with doping

 \rightarrow nesting wavevector increases with PG



Wise, Hudson, Nat Phys 5, 213 (2009)



pseudogap also decreases with doping



Spatial vs. Momentum Resolution



Real space: g(r, E)



0.6% 1st BZ

Superconductivity Tunneling Milestones

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1989: Vortex imaging

Vortex core states (conventional superconductors):

$$E_0 \sim \Delta_{\infty}^2 / E_F$$



Caroli, deGennes, Matricon, Phys. Lett. 9, 307 (1964)



FIG. 2. Abrikosov flux lattice produced by a 1-T magnetic field in NbSe₂ at 1.8 K. The scan range is about 6000 Å. The gray scale corresponds to dI/dV ranging from approximately 1×10^{-8} mho (black) to 1.5×10^{-9} mho (white).



FIG. 3. dI/dV vs V for NbSe₂ at 1.85 K and a 0.02-T field, taken at three positions: on a vortex, about 75 Å from a vortex, and 2000 Å from a vortex. The zero of each successive curve is shifted up by one quarter of the vertical scale.

Hess, PRL 62, 214 (1989)

Vortices in cuprates





Vortex pinning force measurement





Vortex pinning possibilities



(1) no strong pinners
 inter-vortex forces dominate
 → lattice formation



(2) strong pinners exist
 low anisotropy
 → vortices bend slightly
 to accommodate pinners

(3) strong pinners exist
high anisotropy
→ vortices pancake
each pancake pins independently





ideal case for applications



 $Bi_2Sr_2CaCu_2O_8$

NbSe₂

Are Vortices Pinned to Surface Impurities?





Are Vortices Pinned to Surface Impurities?





Idealized Data







0

 \mathbf{O}

Ο

Q

O vortex, radius $\xi_0 = 2.76$ nm

• impurity

→Vortices are <u>not</u> pinned to visible surface impurities

Vortex pinning possibilities



(1) no strong pinners
 inter-vortex forces dominate
 → lattice formation





NbSe₂

(2) strong pinners exist
 low anisotropy
 → vortices bend slightly
 to accommodate pinners

 $Ba(Co_xFe_{1-x})_2As_2$

(3) strong pinners exist
 high anisotropy
 → vortices pancake
 each pancake pins independently





 $Bi_2Sr_2CaCu_2O_8$

Next up: vortices as a window to the "normal" state...