Disorder and quasiparticle interference in high-$T_c$ superconductors

Peter Hirschfeld, U. Florida

$\omega = +2$ meV

P. Choubey, T. Berlijn, A. Kreisel, C. Cao, and P. J. Hirschfeld, Phys. Rev. B 90, 134520

U. Tennessee, 8 February 2016
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Outline

• Unconventional superconductivity
• STM
• Quasiparticle interference
• Bogoliubov-de Gennes + Wannier method
• Applications
  1. Zn impurity in BSCCO
  2. QPI in BSCCO
• QPI as a qualitative tool
How can two electrons attract each other?

Dance analogy: coherent pairs

Another analogy:

J. Robert Schrieffer: “By dancing they lower their energy or make themselves happier”
How Cooper pairs form in conventional superconductors
the “glue”: electron-phonon interaction

Effective “residual” e-e interaction including Coulomb (“Jellium model”)

Realistic system: $a \neq b$! Depends on details

Screened Coulomb Electron-phonon (attraction)

Note: electrons avoid Coulomb repulsion in time (interaction is retarded)
Attraction from repulsion: Kohn-Luttinger 1965

KL: an electron gas with no phonons and only repulsive Coulomb interactions can be a superconductor!

A new paradigm: electrons avoid repulsive part of Coulomb interaction in space rather than time!
At finite distances, screened Coulomb interaction becomes attractive: finite-L pairing
Kohn-Luttinger 1965

Example: short range $U>0$ for rotationally invariant system ($\approx ^3\text{He}$)

$$T_c \approx E_F \exp(-2.5L^4)$$

Best calculation in 1965: Brueckner Soda Anderson Morel PR 1960:

predicted $L=2$ for $^3\text{He}$ $\Rightarrow T_c \sim 10^{-17}\text{K}$

But had they taken $L=1$ they would have gotten $T_c \sim 1\text{mK}$!
Higher – L pair wavefunctions translated into crystalline environment: Symmetry of order parameter $\Delta(k)$ in 1-band superconductor

- **s-wave, L=0** no nodes conventional pair state
- **d-wave, L=2** nodes unconventional pair state
Gap symmetry vs. structure: Important clue to pairing mechanism!

Fe-based superconductors
2 paradigms for superconductivity according to how pairs choose to avoid Coulomb interaction

“conventional”: isotropic s-wave pair wave function, interaction retarded in time

Overall effective interaction attractive

“unconventional”: anisotropic or sign-changing pair wave function,

Overall effective interaction repulsive

Scanning tunnelling microscopy

Tunnelling current:

Local Density Of States (LDOS) of sample at given energy

Conductance $dI/dV$ of FeSe $T_c=8$ K

Topograph of Fe centered impurity in FeSe at $V=6$ mV

LDOS and conductance map: Zn impurity in BSCCO at $V=-2$ mV
Quasiparticle interference ("QPI") experiments

P.T. Sprunger et al, Science 1997

Silver 111 surface

LDOS $\rho(r, \omega)$

$$\rho(q, \omega) = \sum_{L \times L} e^{iq \cdot r} \rho(r, \omega)$$
Quasiparticle interference ("QPI") experiments

- can use a real space probe (STM) to give info about momentum space electronic structure $\varepsilon_{nk}$
- can probe symmetry and structure of superconducting gap function
- relies on *disorder* to provide a signal!
Anderson’s theorem


THEORY OF DIRTY SUPERCONDUCTORS

P. W. Anderson
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 3 March 1959)

Abstract—A B.C.S. type of theory (see Bardeen, Cooper, and Schrieffer, Phys. Rev. 108, 1175 (1957)) is sketched for very dirty superconductors, where elastic scattering from physical and chemical impurities is large compared with the energy gap. This theory is based on pairing each one-electron state with its exact time reverse, a generalization of the \( k \) up, \(-k \) down pairing of the B.C.S. theory which is independent of such scattering. Such a theory has many qualitative and a few quantitative points of agreement with experiment, in particular with specific-heat data, energy-gap measurements, and transition-temperature versus impurity curves. Other types of pairing which have been suggested are not compatible with the existence of dirty superconductors.

In the presence of dirt one can still pair time-reversed members of Kramer’s doublet: thermodynamics (\( T_c \), gap, sp. ht., ...) are not affected by nonmagnetic impurities
Nonmagnetic impurities are pairbreaking in unconventional superconductors
Strong magnetic impurity creates bound state in s-wave SC

BOUND STATE IN SUPERCONDUCTORS WITH PARAMAGNETIC IMPURITIES

Yu Lu

ABSTRACT

A generalized canonical transformation and a SCF method have been used to investigate the influence of isolated impurity atoms on the properties of superconductors. It has been found that a bound state of excitation exists around a paramagnetic impurity with its energy level in the energy gap. An analytical expression has been obtained for the corresponding wave function. The effect of electromagnetic absorption due to the bound state should appear as a precursory peak. The possible experimental verifications of the bound state through tunnelling effect and infrared absorption are discussed.

Furthermore, the excitations of continuous spectra around a nonmagnetic impurity and the spatial variation of the energy gap parameter have been considered.

Yu Lu, Acta Physica Sinica 21, 75 (1965)

see also

Bound states of nonmagnetic impurity in $d$-wave SC

Byers et al (1993):
Local DOS shows 4fold pattern

$\rho(r, \omega) = -\frac{1}{\pi} \text{Im} G(r, r; \omega)$

Balatsky et al. (1995):
Bound state in resonant limit at

$\Omega_0 = \Delta_0 \left( 2N_0u_0 \log 8N_0u_0 \right)^{-1}$

$\delta \rho_{\text{imp}}$

see also Stamp, 1986 (p-wave)
$T_c$ is too high for electron-phonon “glue” to work! What holds pairs together?

\[ \Delta_k = \frac{\Delta_0}{2} (\cos k_x - \cos k_y) \]
Impurities in cuprates

Probe the response of SC to a spin/charge \textit{local perturbation}

\textit{Dilute Cu in-plane substitutions}
- Ni\textsuperscript{2+} 3d\textsuperscript{8} spin 1
- Zn\textsuperscript{2+} 3d\textsuperscript{10} no spin
- Li\textsuperscript{+} no spin
- (Cu?) vacancies

\textit{Out-of-plane dopants: O interstitial, cation switching, …}
$T = 4.2 \text{ K}$

200 pA, -200 mV

$\text{Bi}_2\text{Sr}_2\text{Ca}(\text{Cu}_{1-x}\text{Zn}_x)_2\text{O}_{8+d} : x \approx 0.3\%$

LDOS map at $-1.5\text{mV}$

$\sim 20$

Zn atoms

Zn On-site LDOS spectrum: $W_0=-2$ meV

Compare Zn STM LDOS pattern with simple theory of nonmagnetic impurity in dSC
Compare Zn STM LDOS pattern with simple theory of nonmagnetic impurity in dSC
Theories of impurity resonance spatial pattern


• “Correlations”: Polkolnikov et al 2001, … account for Kondo screening of correlation-induced local moment
“Tunneling involves orbitals that extend out of the planes, such as 4s Cu. These orbitals are symmetric in the Cu-O plane and hence couple to the neighboring metal 3 $d_{x^2-y^2}$ orbitals through the d-wave-like fork”
Bogoliubov-de Gennes (BdG) equations for Cu lattice

\[ H_{MF} = \sum_{ij\mu\nu\sigma} t_{ij}^{\mu\nu} c_{i\mu\sigma}^\dagger c_{j\nu\sigma} - \mu_0 \sum_{i\mu\sigma} c_{i\mu\sigma}^\dagger c_{i\mu\sigma} - \sum_{ij\mu\nu} \left[ \Delta_{ij}^{\mu\nu} c_{i\mu\uparrow}^\dagger c_{j\nu\downarrow}^\dagger + h.c. \right] + \sum_{i^*\mu\sigma} V_{i^*\mu\sigma}^{\mu\nu} c_{i^*\mu\sigma}^\dagger c_{i^*\nu\sigma} \]

\[ \Delta_{ij}^{\mu\nu} = V_{ij}^{\mu\nu} \left\langle c_{j\nu\downarrow} c_{i\mu\uparrow} \right\rangle \]

Applying Bogoliubov transformation leads to BdG equations

\[
\begin{bmatrix}
    t_{ij}^{\mu\nu} - \mu_0 \delta_{ij} \delta_{\mu\nu} \\
    -\Delta_{ij}^{\nu\mu*} \\
    -t_{ij}^{\mu\nu} + \mu_0 \delta_{ij} \delta_{\mu\nu}
\end{bmatrix}
\begin{bmatrix}
    u_{j\nu}^n \\
    v_{j\nu}^n
\end{bmatrix}
= E_n
\begin{bmatrix}
    u_{i\mu}^n \\
    v_{i\mu}^n
\end{bmatrix}
\]

\[ n_{i\mu\uparrow} = \sum_n |u_{i\mu}^n|^2 f(E_n) \quad n_{i\mu\downarrow} = \sum_n |v_{i\mu}^n|^2 (1 - f(E_n)) \]

\[ \Delta_{ij}^{\mu\nu} = V_{ij}^{\mu\nu} \sum_n u_{i\mu}^n v_{j\nu}^* f(E_n) \]

\( u, v \) and \( E_n \) are obtained by solving BdG equations self-consistently for a given filling.
Local Density of States

Lattice Green’s function and Lattice LDOS

\[ G_{ij}^{\mu\nu}(\omega) = \sum_{n\sigma} \left[ \frac{u_{i\mu}^n u_{j\nu}^{*n}}{\omega - E_n + i\eta} + \frac{v_{i\mu}^n v_{j\nu}^{*n}}{\omega + E_n + i\eta} \right] \]

\[ n_{i\mu}(\omega) = -\frac{1}{\pi} \text{Im} [G_{ii}^{i\mu}(\omega)] \]

Local continuum Green’s function and LDOS

\[ G(r, r', \omega) = \sum_{ij\mu\nu} w_{i\mu}(r) G_{ij}^{\mu\nu}(\omega) w_{j\nu}(r')^* \]

\[ w_R(r) = \frac{1}{\sqrt{N}} \sum_k \psi_k(r) e^{-i k \cdot R} \quad \text{(Wannier function for one band system)} \]

\[ A(r, \omega) = -\frac{1}{\pi} \text{Im} [G(r, r, \omega)] \]
Wannier transformation

$$|n\rangle = \sum_{k\nu} e^{-ikr} U_{nj}(k) |k\nu\rangle$$

+ d-wave superconductivity

$$\Delta(k) = \Delta_0 (\cos k_x - \cos k_y)$$

Tight-binding band downfolded
From WIEN2K
Results*: Wannier $d_{x^2-y^2}$ orbital

Cut through $w(r)$ 5Å above plane

Cu- $d_{x^2-y^2}$ Wannier function

Results: Lattice and Continuum LDOS

Lattice LDOS (CuO2 plane)

$v_{imp} = -5 \text{ eV}$

Continuum LDOS (5 Å above BiO surface)

Expt. (Pan et al)

Differential conductance (d$I$/d$V$)

(a) $11 a \approx 41\text{Å}$

BdG

BdG+W

experiment

high

low
Height dependence

Exponential limit
Quasi Particle Interference (QPI)

Simple metal Fermi surface

Cuprate superconductor: Fermi surface and gap
$q_1 \parallel (\pi,0)$

$Hoffman \ et \ al \ (2002), \ McElroy \ (2003)$
“Octet” analysis

qp const. energy contours

\[ n(E) = \left\{ \int_{E(k)=E} \frac{1}{\nabla_k E(\vec{k})} \right\} dk \]
weak impurities

Capriotti et al 2003

\[
|\rho(q)|_\infty |\text{Im }\Lambda(q)| \|u(q)\|
\]

\[
\Lambda(q) \equiv \frac{1}{\pi} \sum_{r \in L \times L} e^{iq \cdot r} G^0(r) G^0(-r)
\]
Critique of 1-impurity and weak scattering analyses:

- Neither can explain peak widths and weights: (100) peaks too small

- Octet peak positions alone give no insight into origins of disorder potential

- Why are peaks so broad in expt.? (no broadening in Capriotti et al analysis)
8% weak potential scatterers, $V_0 = 2t$, range $\lambda = a$,

0.2% unitary scatterers, $V_0 = 30t$,

Zhu Atkinson PH 2004
QPI simulation of continuum LDOS 5Å above plane

BSCCO: weak potential scatterer

spots from octet model

Fourier transform

no intra-unit cell information

atomic scale local density of states at STM tip position

full information for all scattering vectors

no information beyond first BZ

atomic scale local density of states at STM tip position
BdG+Wannier: 
THE MOVIE
Comparison to experiment

no large q information

relative conductance map, Fourier transformation

energy integrated relative conductance maps

K Fujita et al. Science 344, 612 (2014)
QPI as a model-free phase-sensitive tool in unconventional superconductors


1. QPI is not...
   - a quantitative tool
   - a low-energy (near-Fermi) property
   - proportional to coherence factors

2. But QPI may be
   - a qualitative tool, if one can see qualitatively different behavior in different cases of interest (e.g., $s_\pm$ vs. $s_{++}$)
1. QPI is not
   - a quantitative tool
     e.g. Hänke et al. PRL 2012
   - proportional to coherence factors

<table>
<thead>
<tr>
<th>Scatterer</th>
<th>$C(q)$ in $R^{odd}(q, V)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weak scalar</td>
<td>$(uu' - vv')^2$</td>
</tr>
<tr>
<td>Weak magnetic</td>
<td>0</td>
</tr>
<tr>
<td>Resonant</td>
<td>$(uu' + vv')(uu' - vv')$</td>
</tr>
<tr>
<td>Andreev</td>
<td>$(uu' - vv')(uu' + vv')$</td>
</tr>
</tbody>
</table>

Maltseva & Coleman, 2009
QPI as a model-free phase-sensitive tool

Chi et al, PRB 2014

Does superconductivity enhance the large $q$ transitions and suppress the small $q$ ones?

LiFeAs

Qualitative probe of gap sign change?
Chi et al. 2014

Assuming

\[
W_{i \to f}(k, k') \propto |u_i(k)u_f^*(k') \pm v_i(k)v_f^*(k')|^2 \\
\times |V(k' - k)|^2 N_i(k)N_f(k'),
\]

Theory: PH, Altenfeld, Eremin, Mazin PRB 2015
Conclusions

1. Simple method of using discarded Wannier function information to calculate local STM conductance in inhomogeneous SC: enhances resolution, preserves local symmetries, allows calculation of true surface properties.

2. Application to BSCCO: resolution of old Zn and Ni paradoxes
   Dramatic improvement of QPI calculations

3. Suggestions to determine gap signs: (i) s/c-normal differences and (ii) symmetized/antisymmetrized combinations are more informative than just QPI. (iii) monitor T-dependence at a given bias
Coherence factors

\[ |Z(q, E)|^2 \propto \left[ \frac{2\pi}{\hbar} \int \frac{dE'}{E - E'} \int dk_1 dk_2 C(k_1, k_2) t_{k_1, k_2} \delta(E - E_{k_1}) \delta(E' - E_{k_2}) \delta^{(2)}(k_1 - (k_2 + q)) \right]^2 \]

\[ C(k_i, k_f) = (u_{k_i} u_{k_f} - v_{k_i} v_{k_f})^2 \]

Hanaguri et al 2008, Maltseva and Coleman 2009

\[ W_{i \rightarrow f}(k, k') \propto |u_i(k)u^*_f(k') \pm v_i(k)v^*_f(k')|^2 \times |V(k' - k)|^2 N_i(k) N_f(k'), \]

Chi et al 2014
FTLDOS for single impurity

\[
\delta \rho(q, \omega) = \frac{1}{\pi} \text{Im} \sum_k \left[ \hat{G}^0(k, \omega) \hat{t}(\omega) \hat{G}^0(k + q, \omega) \right]_{11}
\]

\[
= \frac{1}{2} \text{Tr} \text{Im} \sum_k (\tau_0 + \tau_3) \hat{G}^0(k, \omega) \hat{t}(\omega) \hat{G}^0(k + q, \omega).
\]

Small q integrated weight:

\[
\delta \rho_{\text{intra}}(\omega) = \frac{1}{2} \text{Tr} \text{Im} \sum_{k, q \approx 0, \nu} (\tau_0 + \tau_3) \hat{G}_{\nu}^0(k, \omega) \hat{\nu}(\omega) \hat{G}_{\nu}^0(k + q, \omega)
\]

\[
\approx \frac{1}{2} \text{Tr} \text{Im} \sum_{k, q, \nu} (\tau_0 + \tau_3) \hat{G}_{\nu}^0(k, \omega) \hat{t}_{\nu \nu}(\omega) \hat{G}_{\nu}^0(k + q, \omega)
\]

\[
= \frac{1}{2} \text{Tr} \text{Im} \sum_{k, k', \nu} (\tau_0 + \tau_3) \hat{G}_{\nu}^0(k, \omega) \hat{t}_{\nu \nu}(\omega) \hat{G}_{\nu}^0(k', \omega),
\]

Independent k sums: use \(
\sum_k \hat{G}_{\nu}^0(k, \omega) \approx i \pi \rho_{\nu} \frac{\omega \tau_0 + \Delta_{\nu} \tau_1}{\sqrt{\omega^2 - \Delta_{\nu}^2}}.
\)

Similarly for interband terms...
Determine $\Delta$ sign change by measuring symmetrized and antisymmetrized conductances at large and small $q$

\[ \rho_{\text{intra}}^{(\pm)}(\omega) = \rho_{\text{intra}}(\omega) \pm \rho_{\text{intra}}(-\omega), \]

<table>
<thead>
<tr>
<th>Channel</th>
<th>$s_{++}$</th>
<th>$s_{\pm}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta \rho^{(+)}$</td>
<td>$\checkmark$</td>
<td>$\checkmark$</td>
</tr>
<tr>
<td>$\delta \rho^{(-)}$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>$\delta \rho^{(-)}$</td>
<td>$\checkmark$</td>
<td>$\times$</td>
</tr>
</tbody>
</table>

**TABLE I.** Presence or absence of singular response in the symmetric ($+$) and antisymmetric ($-$) channels for $s_{++}$ and $s_{\pm}$ superconductors of the integrated QPI intensity (Fourier transformed density of states). Here $\checkmark$ indicates the presence of a strong frequency dependent response in the given channel, and the $\times$ indicates the absence of one.

T-dependence as one enters SC state should be most sensitive measure!
Remark on “Hanaguri method”

- M. Maltseva and P. Coleman, PRB 80, 144514 2009: formalism with coherence factors
- T. Hanaguri et al Science 328, 474 (2010): same for Fe(Se,Te)

Pereg-Barnea and Franz 2008

It then follows that

$$\delta n_e(q_{ij}, \omega) \sim \begin{cases} 4\omega^2 K_{ij} (\omega), & \text{if } \text{sgn} \Delta_i = \text{sgn} \Delta_j \\ 0, & \text{if } \text{sgn} \Delta_i \neq \text{sgn} \Delta_j \end{cases}$$

(15)

Thus, remarkably, we find that only those interference peaks will be enhanced by applied magnetic field whose wavevectors $q_{ij}$ connect octet points in the regions of the Brillouin zone with the same sign of the gap function $\Delta_k$, denoted by $+/+$ and $-/-$ in Fig. 1(a). These are $q_1$, $q_4$, and $q_5$. The remaining $+/-$ peaks will be to leading order unaffected. The resulting pattern is illustrated in Fig. 1(b). We remark that these are precisely the peaks observed to be enhanced in the experiments by Hanaguri et al. 9.

No real theoretical understanding of why field suppresses $-+$ q vectors
Emergent defect states: theory 1. SDW state

Gastiasoro, PJH, and Andersen, PRB 2013

\[
H = H_0 + H_{int} + H_{imp},
\]

\[
H_0 = \sum_{i,j,\mu,\nu,\sigma} t_{ij}^{\mu\nu} c_{i\mu\sigma}^\dagger c_{j\nu\sigma} - \mu_0 \sum_{i,\mu,\sigma} n_{i\mu,\sigma}
\]

\[
H_{int} = U \sum_{i,\mu} n_{i\mu\uparrow} n_{i\mu\downarrow} + (U' - J) \sum_{i,\mu < \nu, \sigma < \sigma'} n_{i\mu\sigma} n_{i\nu\sigma'}
\]

\[
- 2J \sum_{i,\mu < \nu} \vec{S}_{i\mu} \cdot \vec{S}_{i\nu} + J' \sum_{i,\mu < \nu, \sigma} c_{i\mu\sigma}^\dagger c_{i\mu\sigma'}^\dagger c_{i\nu\sigma'} c_{i\nu\sigma},
\]

\[
H_{imp} = V_{imp} \sum_{\mu,\sigma} c_{i\mu\sigma}^\dagger c_{i\mu\sigma}
\]

\[
H_{ij\sigma}^{\mu\nu} = t_{ij}^{\mu\nu} + \delta_{ij} \delta_{\mu\nu} [-\mu_0 + \delta_{i\mu} V_{imp} + U \langle n_{i\mu\bar{\sigma}} \rangle + \sum_{\mu' \neq \mu} (U' \langle n_{i\mu'\bar{\sigma}} \rangle + (U' - J) \langle n_{i\mu'\sigma} \rangle)]
\]
“Nematogens” grow as $T$ lowered: magnetization

Origin of electronic dimers in the SDW phase

**Magnetization**

(a) (d)

**Density**

(b) (e)

**LDOS**

(c) (f)

**FIG. 3.** (Color online) 2D real-space maps of (a,d) the magnetization, (b,e) the total electron charge density, and (c,f) the low-energy integrated LDOS for the same two low-$T$ nematogens shown in Fig. 2(d,h).
Emergent defect states: theory 2. “Nematic state” $T_N < T < T_S$

“$t_x/t_y$” = 1.05
$V_{imp} = 6\text{eV}$

$Ishida et al 2013$

$T/T_N = 1.43$

$T/T_N = 1.29$

$T/T_N = 1.21$

$T/T_N = 1.14$

$T/T_N = 1.07$
Scattering rate anisotropy

Self-consistent BdG

\[ \langle k'\nu\sigma|V^{\text{imp}}|k\mu\sigma\rangle = \langle k'\nu\sigma|\mathcal{H} - \mathcal{H}_0|k\mu\sigma\rangle \]

\[ \frac{1}{\tau_{k\alpha}} = n_{\text{imp}} \frac{2\pi}{\hbar V} \frac{1}{V} \sum_{k'\beta} \left| \text{tr} \left( \hat{\sigma}_i \hat{V}^{\text{imp}}_{\sigma\sigma'}(k\alpha, k'\beta) \right) \right|^2 \]

\[ \delta(\epsilon_{k\alpha} - \epsilon_{k'\beta}) \left( 1 - \frac{v^\alpha_F(k) \cdot v^\beta_F(k')}{|v^\alpha_F(k)||v^\beta_F(k')|} \right), \]

5% band structure anisotropy \( \Rightarrow \) 250% anisotropy in scattering rate!

spin fluctuation enhancement of impurity potential anisotropy
Scattering rate in $b$ direction “diverges” at $T_N$.

Gastiasoro et al. aXv:1407.0117
Summary of results

- Small fixed strain
- Tetragonal phase
- Ortho
- "Tetragonal"
- $x \sim 0.02$

SDW $T_n$, $T_s$, $T$

Controlled strain (tetragonal phase)
Summary of results

- **small fixed strain**
- **SDW**
- **$T_nT_s$**
- **$T$**
- **controlled strain**
  - (tetragonal phase)

- **ortho**
- **“tetragonal”**

- $x \sim 0.02$

- $\rho_b$
- $\rho_a$

- $\varepsilon_{yy}$
### Summary of results

- **Small fixed strain**
  - SDW
  - $T_n T_s$
  - **Ortho**
  - "Tetragonal"

- **Controlled strain** (tetragonal phase)
  - $\varepsilon_{yy}$
  - $\rho_b$
  - $\rho_a$
  - $x \approx 0.02$
Generalization to strong scatterers \((\text{Zhu et al 2003})\)

\[
\delta \rho(q) = - \frac{1}{\pi} \sum_{\alpha=0...3} t_\alpha(q) \text{Im}[e^{i\phi_\alpha} \Lambda_\alpha(q)]
\]

**t-matrix for 1 zero range impurity**  
\[ t_\alpha(q) = t_\alpha \sum_i e^{iq \cdot R_i}; \]

**phase of 1-imp. t-matrix**  
\[ \Lambda_\alpha(q) = \sum_k G^0(k, \omega) \tau_\alpha G^0(k + q, \omega) \]

\(\alpha=3\): “potential scatt.”  \(\alpha=0\): “magnetic scatt.”

\[ \delta \rho \text{ still } = (\text{octet peaks}) \bullet (\text{noise}) \]

No broadening in q-space **unless** scattering is **not weak and not zero range**
Why QPI is not a quantitative tool?

- What is measured?
  tunneling conductance $g(r, E)$, which is related to the local DOS $\rho(r, E)$
  related it is...

$\rho(r, E) \sum_k \text{Im}[\tau_3 G(k + q, E - i\delta)t_{k+q,k} G(k, E - i\delta)]$

$t = (a + bi)\tau_3 + (c + di)\tau_0$

- It is not a low-energy (near-Fermi) property

$\int \frac{dE'}{E - E'} \int dk_1dk_2 C(k_1, k_2) t_{k_1,k_2} \delta(E - E_{k_1})\delta(E' - E_{k_2})\delta^{(2)}(k_1 - (k_2 + q))$

It is not proportional

$E_{k}^2 \neq E_k E_{k'}$

$Tr \text{Im} \int_k \tau_3 G_k(\omega)\tau_3 G_{k+q}(\omega)$

$\int_k (E^2 + \xi_k \xi_{k+q} - \Delta_1 \Delta_2) \text{Im} \frac{1}{E^2 - E_k^2} \text{Re} \frac{1}{E^2 - E_{k+q}^2}$
Ab initio evidence for weak normal state filter:

(Wang, Cheng, PH PRB 2004)

1.5Å above surface

Cu-O plane

Q: How to include SC?
Ni impurity in BSCCO: expt.*

\[ \Omega = +9 \text{ meV} \]

\[ \Omega = -9 \text{ meV} \]

*Hudson et al., Nature 403, 786 (2000)
Magnetic impurity in BdG

Ni has $3d^8$ configuration which leads to magnetic moment on the impurity site ($S=1$). Approximating it as a classical spin:

$$H_{imp}^{\text{mag}} = J(n^\uparrow_i - n^\downarrow_i)$$

=> Electrons with spin up and down see effective impurity potentials $V_{imp} + J$ and $V_{imp} - J$ respectively.

Spin-up resonance $\Omega = \pm 2.4$ meV

Spin-down resonance $\Omega = \pm 7.2$ meV

$V_{imp} = 0.625$ eV
Results*: Lattice and Continuum LDOS

\[ \Omega = 2.4 \text{ meV} \]

\[ \Omega = -2.4 \text{ meV} \]

* Manuscript under preparation
Results: Lattice and Continuum LDOS

BdG

BdG+W

Experiment

Impurity

NN

NNN

Far away
V- vs U- shape LDOS spectra

Underdoped cuprates show clean V-shape d-wave like spectrum
Optimal-overdoped cuprates show “U-shaped” spectrum – why?


BdG+W LDOS gives spectra resembling U-shape. What will happen if strong correlations are included?
Nonlocal contributions to local continuum Green’s function

Wannier function above surface

homogeneous case:

\[ G_{RR'}(\omega) = \sum_k G(k, \omega) e^{ik \cdot (R-R')} \]

\[
G(r, r', \omega) = \sum_{\substack{RR' \ni RR' \ni \omega}} G_{RR'}(\omega) w_R(r) w_{R'}(r)^* \\
= \sum_k G(k, \omega) |w_k(r)|^2
\]

where

\[
w_k(r) = \sum_k w_R(r) e^{ik \cdot R}
\]

\[
\approx a_0(r) + a_1(r)[\cos k_x - \cos k_y] + a_2(r)[\cos 2k_x - \cos 2k_y] + \\
a_3(r)[\cos 2k_x \sin k_y - \cos 2k_y \sin k_x] + ...
\]
Wannier analysis: implications for “filter” mechanism

\[ w_k(r) = \sum_k w_R(r) e^{ik \cdot R} \]
\[ \approx a_0(r) + a_1(r)[\cos k_x - \cos k_y] + a_2(r)[\cos 2k_x - \cos 2k_y] + a_3(r)[\cos 2k_x \sin k_y - \cos 2k_y \sin k_x] + \ldots \]

\[ G(r, r', \omega) = \sum_k G(k, \omega) |w_k(r)|^2 \]
\[ \approx \sum_k G(k, \omega) |a_0(r)|^2 + \sum_k G(k, \omega) |a_1(r)|^2 (\cos k_x - \cos k_y)^2 \]
\[ + \sum_k G(k, \omega) |a_2(r)|^2 (\cos 2k_x - \cos 2k_y)^2 + \ldots \]
\[ \approx |a_0(r)|^2 \frac{\omega}{\Delta_0} + |a_1(r)|^2 \left( \frac{\omega}{\Delta_0} \right)^3 + O(\omega)^5 + \ldots \] (interference terms vanish)

Conclude: linear-\(\omega\) contribution to LDOS comes from local piece of \(w(r)\)
Any purely NN “filter” tunneling mechanism (Balatsky, Ting) yields \(\omega^3\) only
Effective Wannier function range may shrink with correlations
Iron-based superconductors

Recent reviews: Stewart RMP 2012; Paglione & Greene Nat Phys 2010

LaFeAsO

$T_c=28K$
(55K for Sm)

BaFe$_2$As$_2$
- Rotter et al, PRL (2008)

$T_c=38K$

LiFeAs

$T_c=18K$

FeSe
- Hsu et al, PNAS 2008

$T_c=8K$

No arsenic 😊!
STM: emergent defect states

Those shown believed to be Fe vacancies or substituents (J.E. Hoffman)

Zhou, PRL 106, 087001 (2011)

Hanaguri, unpublished

Song, Science 332, 1410 (2011)
STM: exotic local defect states

1. Geometric dimer
2. Electronic dimer

FeSe on graphite, Song et al., PRL 109, 137004 (2012)
Results*: Wannier orbitals

$d_{xy}$ Wannier orbitals on two Fe atoms in unit cell

Results FeSe: Lattice LDOS

LDOS far from impurity site, at impurity sites and at NN and NNN sites to impurity.

DOS in homogeneous system

Bound states at $\omega = \pm 8$ meV for 5 meV impurity potential
Results FeSe: Lattice & continuum LDOS maps

Real space patterns of lattice LDOS at 8 meV

xy- cuts through continuum LDOS(x,y,z; \( \omega \)) at different heights z from Fe plane.

C\(_4\) symmetry intact in Fe plane

Dimer like structures obtained above Se plane
Comparison of experimental topograph at 6 meV set-point bias (a) with BdG only (b) and BdG+W LDOS (c)