Discussion on FT-IETS and Bosonic Function in High-Tc Superconductors

A.V. Balatsky

Motivation:

$\alpha^2(\vec{q},\Omega)F(\vec{q},\Omega)$

- Spectroscopy technique
- Properties of electron-boson interaction at nanoscale in real-space: local/delocalized ?
- For anisotropic electron-boson interaction, measure directly momentum transfer $\vec{q}$ and energy Ω_0
- Ideally find the anisotropic electron-boson spectral density

Collaborators:
J.X. Zhu, A. Abanov(LANL)
Q. Si(Rice), Jinho Lee, Kyle McElroy, JC Davis(Cornell)

Old results

VOLUME 17, NUMBER 22 PHYSICAL REVIEW LETTERS 28 NOVEMBER 1966

MOLECULAR VIBRATION SPECTRA BY ELECTRON TUNNELING

R. C. Jaklevic and J. Lambe
Scientific Laboratory, Ford Motor Company, Dearborn, Michigan
(Received 18 October 1966)

The conductance of metal–metal oxide–metal tunneling junctions has been observed to increase at certain characteristic bias voltages. These voltages are identified with vibrational frequencies of molecules contained in the barrier.

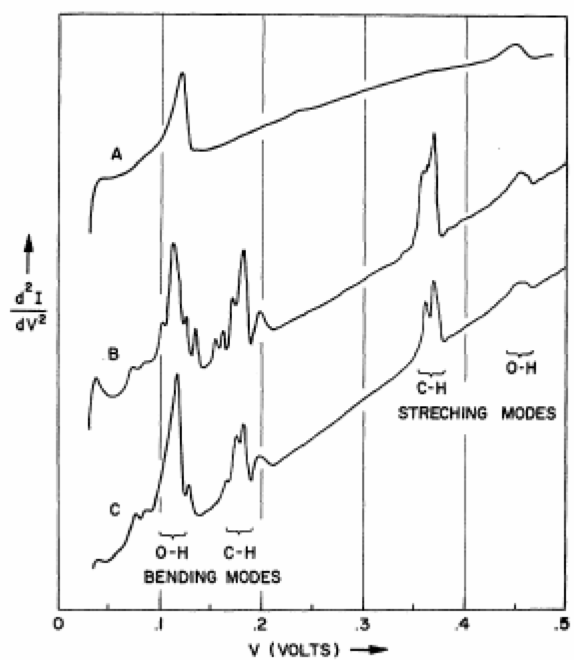
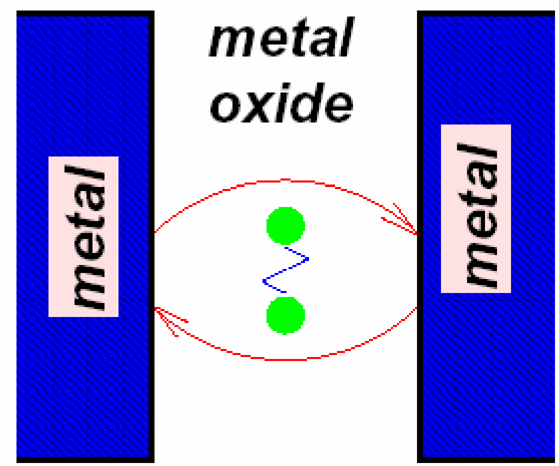


FIG. 1. Recorder traces of d^2I/dV^2 versus applied



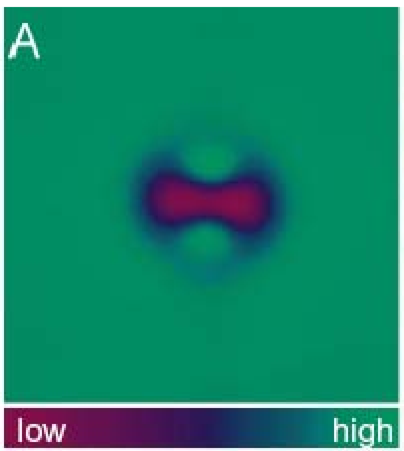
- $H_t = c_L^\dagger c_R T(x) + h.c.$
- $T(x) = t_0(1 + \alpha x)$
- x – Vibrational mode

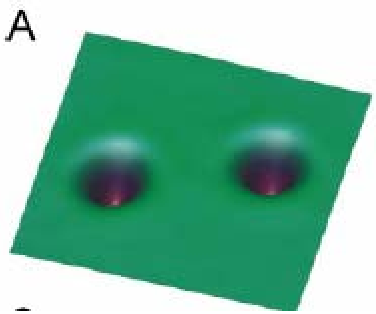
First STM observation of local inelastic scattering mode

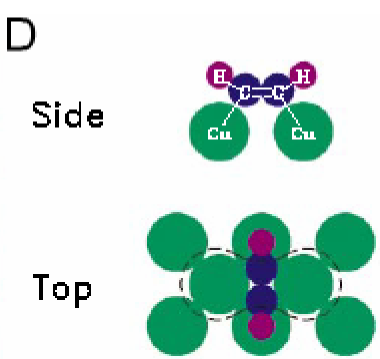
Single-Molecule Vibrational Spectroscopy and Microscopy

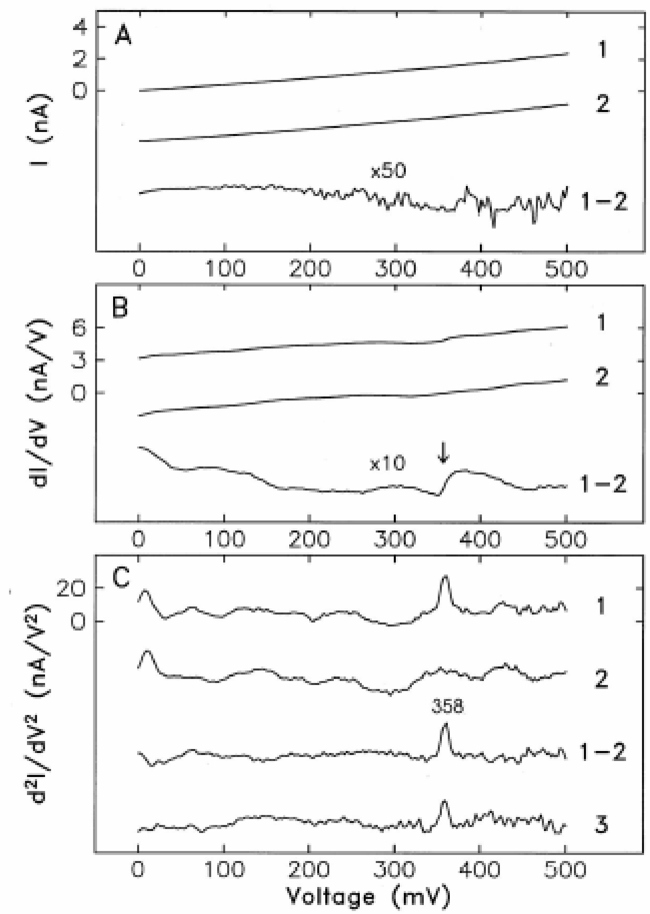
B. C. Stipe, M. A. Rezaei,

SCIENCE • VOL. 280 • 12 JUNE 1998

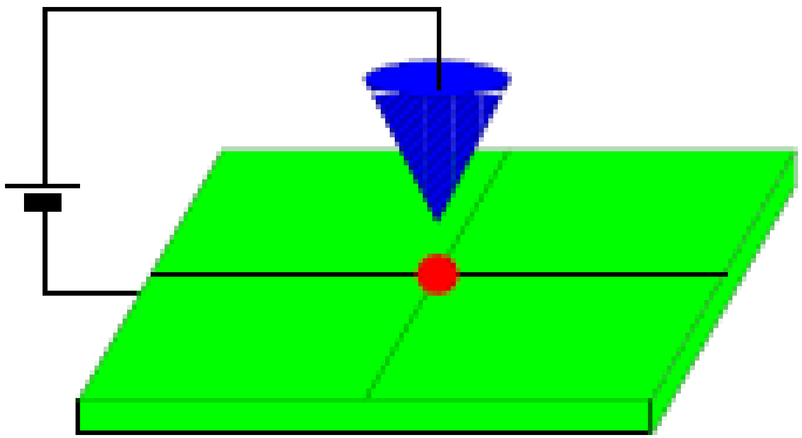








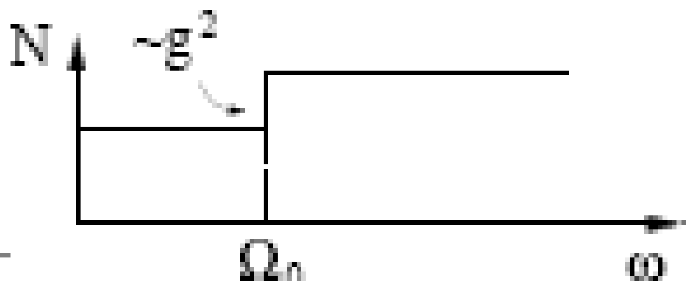
Inelastic STM



- STM measures local DOS
- $H = H_e + H_v + H_i$
- $H_v = \frac{kx^2}{2}$ – vibrational mode
- $H_i = g c_\sigma^\dagger(\mathbf{r}=0) c_\sigma(\mathbf{r}=0) x$

$$\delta N(\omega) = \frac{1}{\pi} \mathrm{Im}\left[G^0(\mathbf{r},\omega) \Sigma(\omega) G^0(\mathbf{r},\omega) \right]$$

For normal metal: $\delta N(\omega) \sim g^2 N_0(\omega - \Omega_0)\theta(\omega - \Omega_0)$



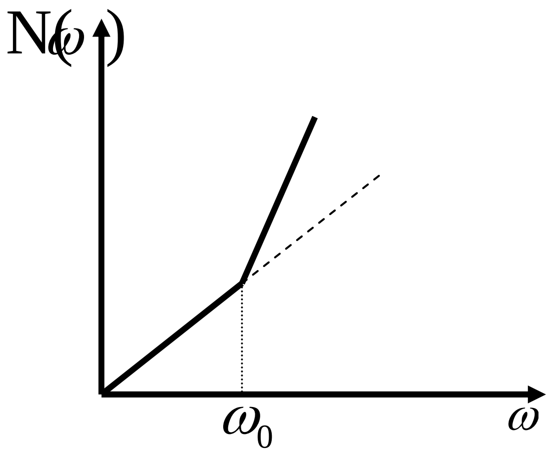
Second order analysis

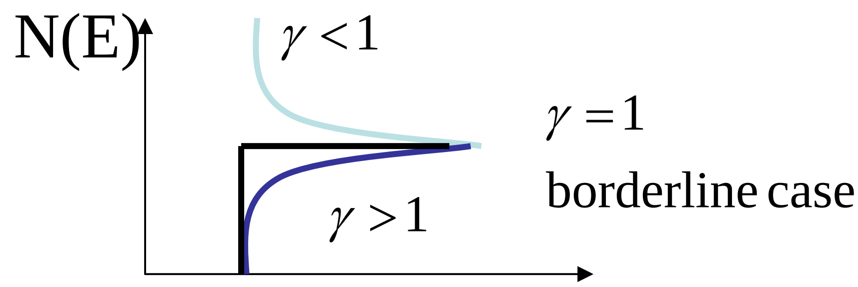
For a d-wave or a pseudo-gapped state feature will be much smaller

$$\delta N(\mathrm{r},\omega) \sim \mathrm{g}^2(\omega-\Omega_0)^{\gamma}\,\Theta(\omega-\Omega_0)$$

where γ is the DOS power

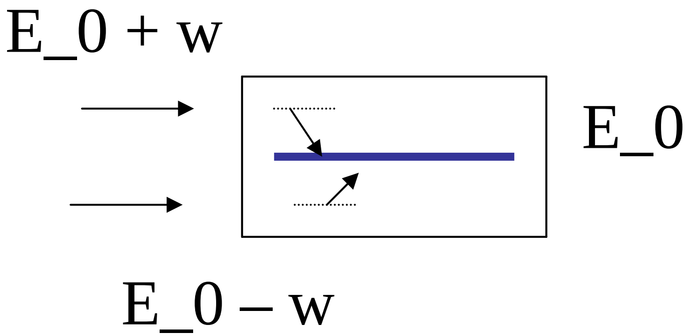
[redacted]



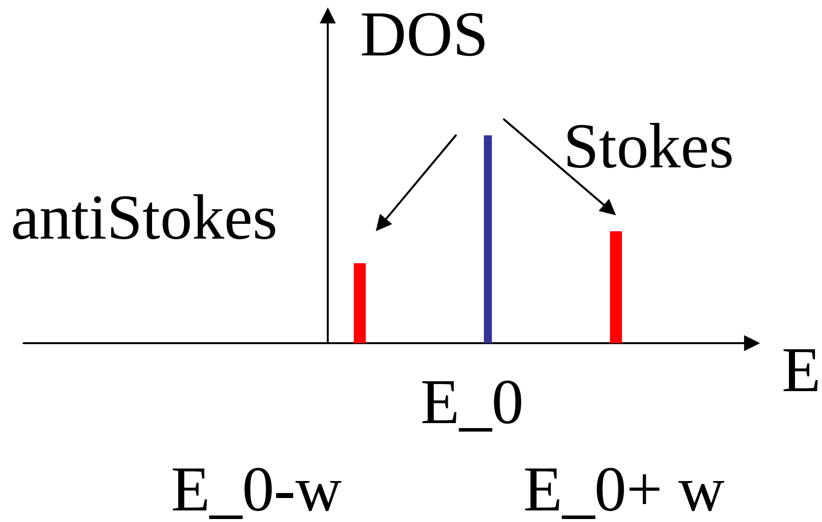


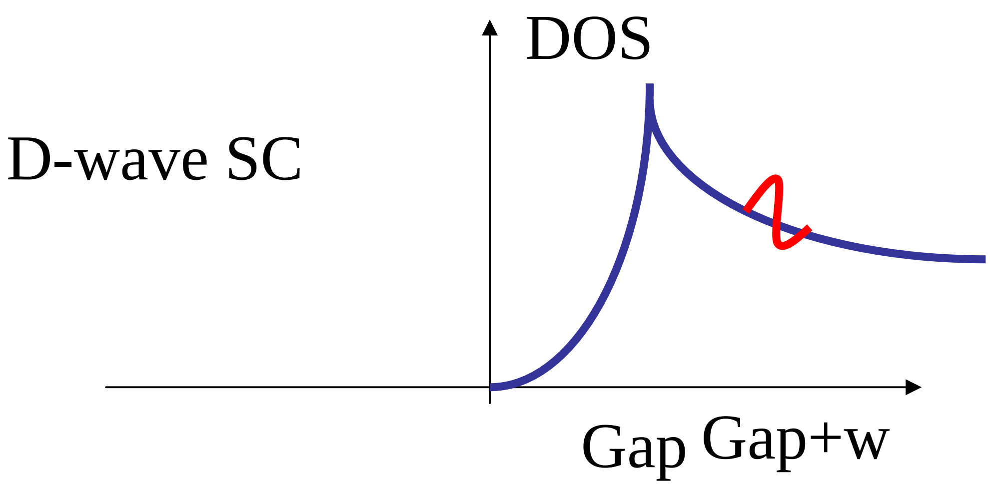
Similar to x-ray absorption singularity

Inelastic scattering induced satellites: Holstein effects

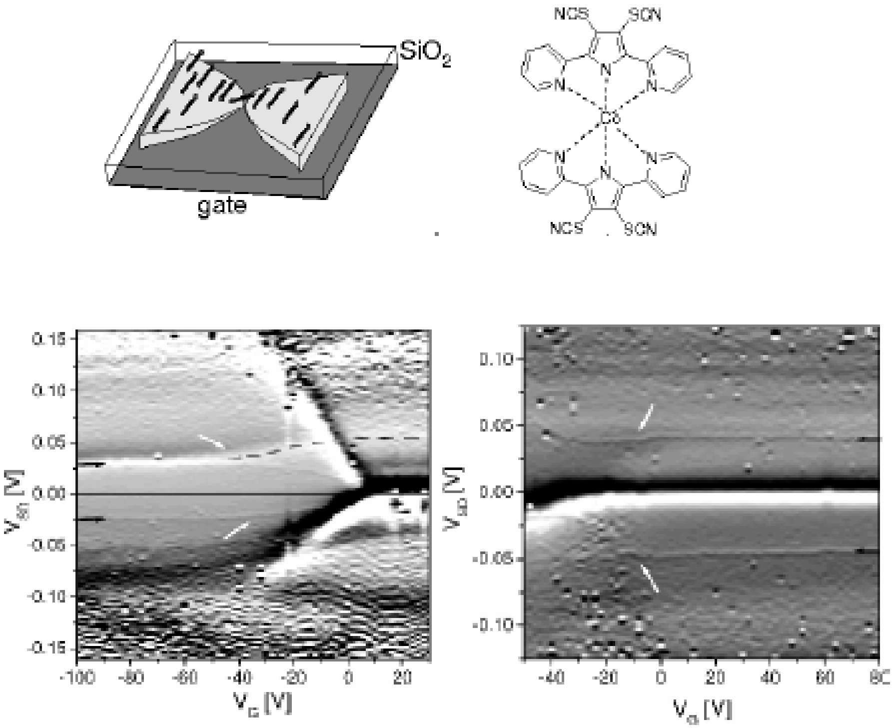


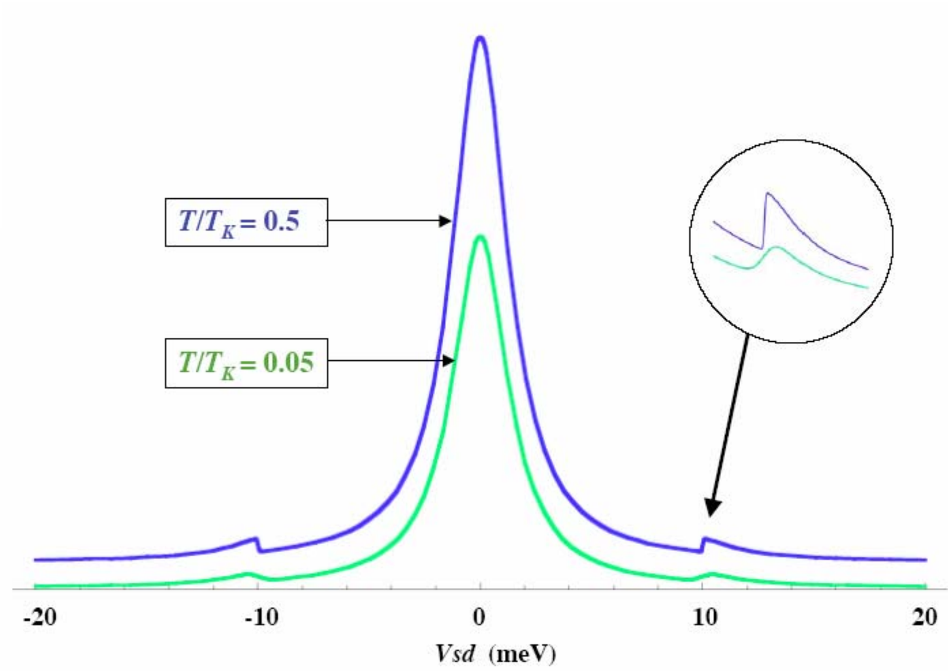
At finite T there is a probability that local mode is excited





Inelastic satellites to Kondo peak in molecular devices





D. Natelson et al, cond-mat 0408052

Abrahams and AVB, preprint

Inelastic Tunneling Spectroscopy in a D-wave Superconductor.

A.V. Balatsky, Ar. Abanov, and Jian-Xin Zhu

PRB, sept 2003

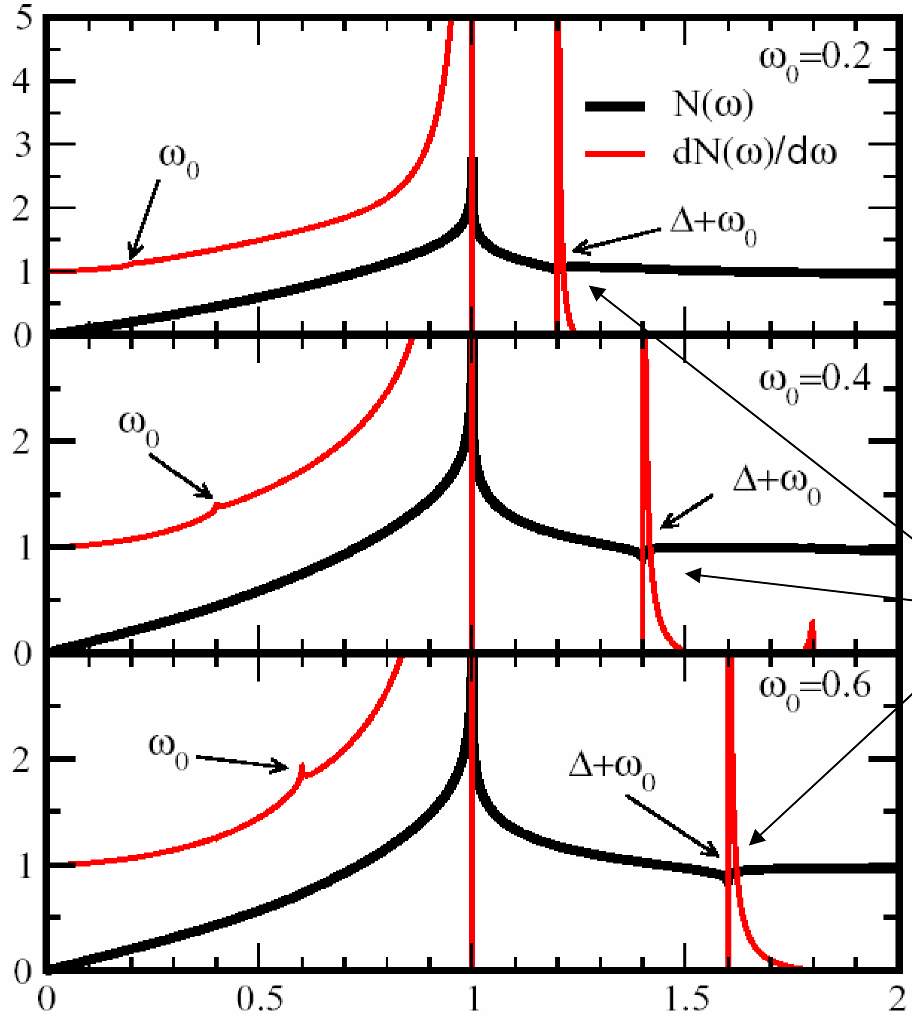
$$H = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma}\epsilon(\mathbf{k})c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}}(\Delta(\mathbf{k})c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow} + h.c.) + \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} J\mathbf{S}\cdot c^{\dagger}_{\mathbf{k}\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{\mathbf{k}'\sigma'} + g\mu_B\mathbf{S}\cdot\mathbf{B}\,,$$

$$\Sigma(\omega_l) = J^2T\sum_{\mathbf{k},\Omega_n} G(\mathbf{k},\omega_l-\Omega_n)\chi^{+-}(\Omega_n)$$

$$\frac{\delta N(\mathbf{r}=0,\omega)}{N_0} = \frac{\pi^2}{2}(JSN_0)^2\frac{\omega-\omega_0}{\Delta}K(T,\omega,\omega_0) \times\left(\frac{2\omega}{\Delta}\ln\left(\frac{\Delta}{\omega}\right)\right)^2,\quad \omega\ll\Delta\,, \tag{6}$$

$$\frac{\delta N(\mathbf{r}=0,\omega)}{N_0} = 2\pi^2(JSN_0)^2K(T,\omega,\omega_0)\ln^2\left(\frac{|\omega-\Delta|}{4\Delta}\right) \times\ln\left(\frac{4\Delta}{|\omega+\omega_0-\Delta|}\right) + (\omega_0\to-\omega_0),\ \omega\simeq|\Delta|\,, \tag{7}$$

Selfconsistent solution for a local vibrational mode



Black line - DOS

Red line- DOS derivative

For $N_0 \sim 1/eV, JN_0 = 0.14$

$$\frac{\delta N}{N_0} \sim (JN_0)^2 \frac{\omega - \Omega_0}{\Delta_0}$$

Holstein features

For relative change compared to d-wave DOS effect is few percent

Inelastic Tunneling Spectroscopy in a D-wave Superconductor.

A.V. Balatsky, Ar. Abanov, and Jian-Xin Zhu

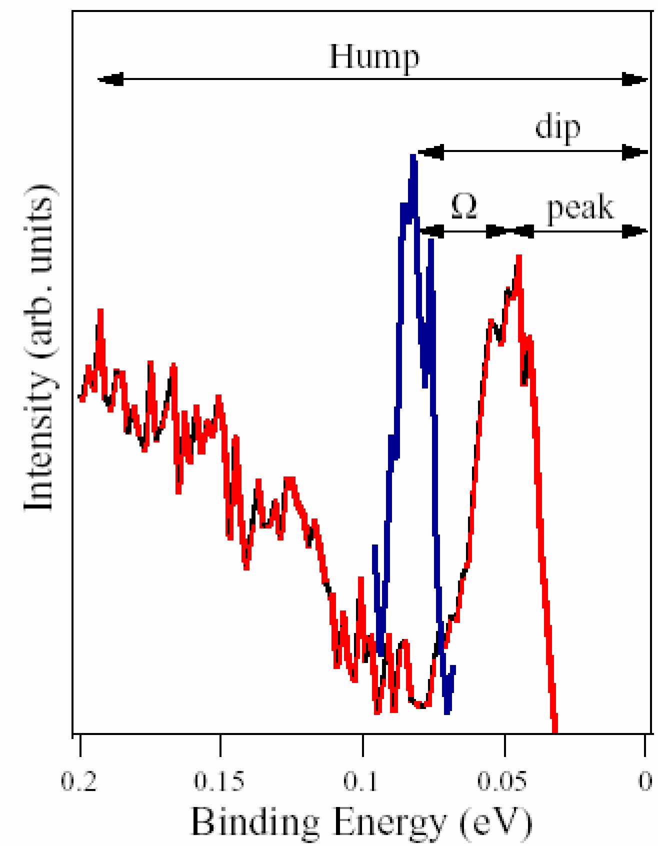
PRB 68 214506 (2003).

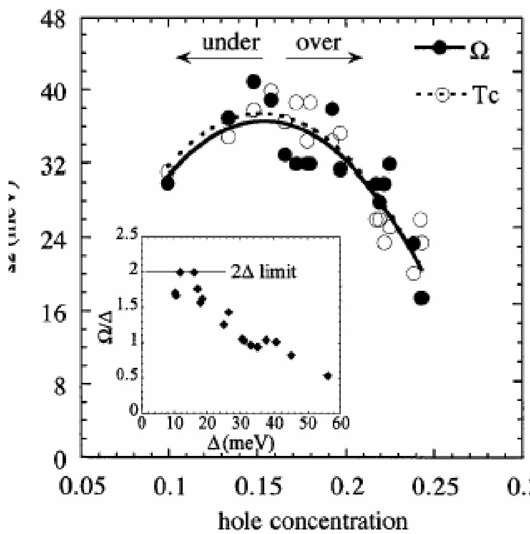
Previous Tunneling work

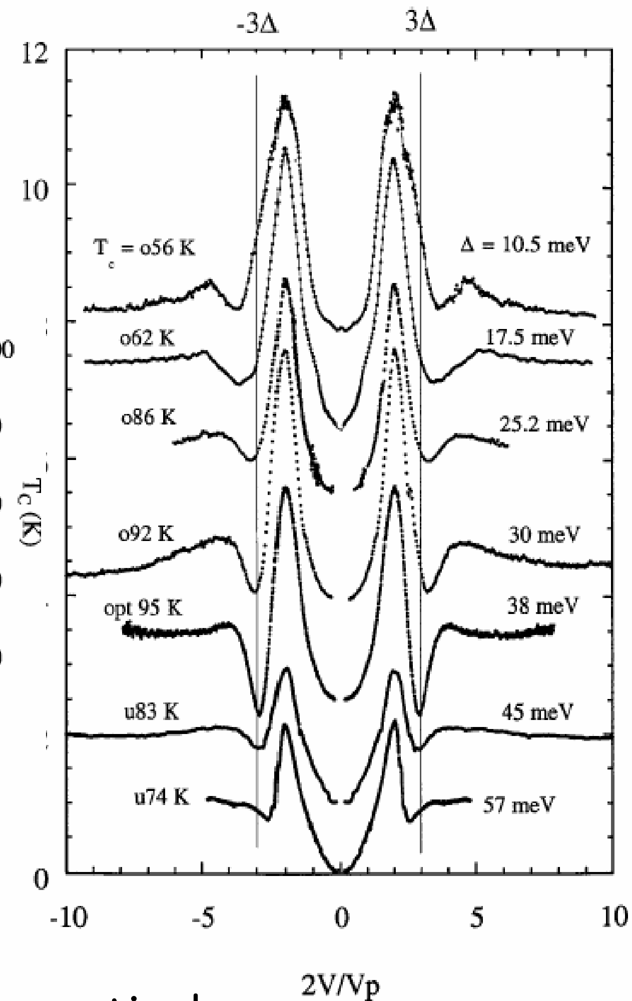
Correlation of Tunneling Spectra in $Bi_2Sr_2CaCu_2O_{8+\delta}$ with the Resonance Spin Excitation

J. F. Zasadzinski,[1,2] L. Ozyuzer,[2,3] N. Miyakawa,[4] K. E. Gray,[2] D. G. Hinks,[2] and C. Kendziora[5]

M. Norman *et al*, PRL., **79**, 3506 (1997)







$\alpha^2 F(\omega)$

But no real-space or q-space information!

Model and formalism

$$\mathcal{H} = \mathcal{H}_{BCS} + \mathcal{H}_{cp} + \mathcal{H}_{imp}$$

$$\mathcal{H}_{BCS} = \sum_{\mathbf{k},\sigma}(\varepsilon_{\mathbf{k}} - \mu)c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}}(\Delta_{\mathbf{k}}c^{\dagger}_{-\mathbf{k}\downarrow}c^{\dagger}_{\mathbf{k}\uparrow} + \Delta^{*}_{\mathbf{k}}c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow})$$

$$\mathcal{H}_{cp} = g\sum_i \mathbf{S}_i \cdot \mathbf{s}_i$$

$$\mathcal{H}_{imp} = U_0 \sum_\sigma c^{\dagger}_{0\sigma}c_{0\sigma}$$

Model and formalism (cont'd)

Bare GF: $\widehat{G}_0^{-1}(\mathbf{k}; i\omega_n) = \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & i\omega_n + \xi_{\mathbf{k}} \end{pmatrix}$.

Self energy: $\hat{\Sigma}(\mathbf{k}; i\omega_n) = \frac{g^2 T}{8N} \sum_{\mathbf{q}} \sum_{\Omega_l} \chi(\mathbf{q}; i\Omega_l) \begin{pmatrix} 3G_{0,11} & G_{0,12} \\ G_{0,21} & 3G_{0,22} \end{pmatrix} (\mathbf{k}-\mathbf{q}; i(\omega_n - \Omega_l))$.

Dressed GF: $\underline{\widehat{G}}_0^{-1}(\mathbf{k}; i\omega_n) = \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} - \Sigma_{11} & \Delta_{\mathbf{k}} - \Sigma_{12} \\ \Delta_{\mathbf{k}} - \Sigma_{21} & i\omega_n + \xi_{\mathbf{k}-\Sigma_{22}} \end{pmatrix}$.

Model and formalism (cont'd)

Site-dependent GF (TMA) w/ imp:

$$\widehat{G}(i,j;E) = \underline{\widehat{G}}_0(i,j;E) + \underline{\widehat{G}}_0(i,0;E)\hat{T}(E)\underline{\widehat{G}}_0(0,j;E)$$

$$\hat{T}^{-1} = U_0^{-1}\sigma_3 - \underline{\hat{g}}_0, \; \underline{\hat{g}}_0(i\omega_n) = \underline{\widehat{G}}_0(i,i;i\omega_n)$$

LDOS: $\rho_i(E) = -\frac{2}{\pi}\mathrm{Im}G_{11}(i,i;E+i\gamma)$.

Band DOS ($U_0 = 0$): $\rho(E) = \sum_{\mathbf{k}} A_{\mathbf{k}}(E)$. $A_{\mathbf{k}}(E) = -\frac{2}{\pi}\mathrm{Im}\underline{G}_{0,11}(\mathbf{k};E+i\gamma)$.

Numerical results and discussions

Parameter values: $t = 1.0$, $t' = -0.2$ $[\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y]$

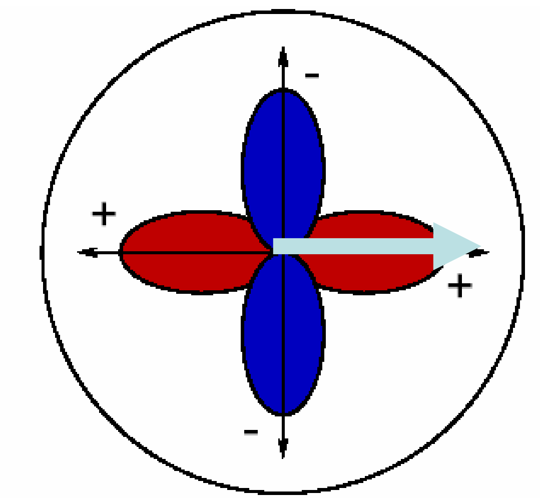
$\Delta_0 = 0.1$ $[\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)]$

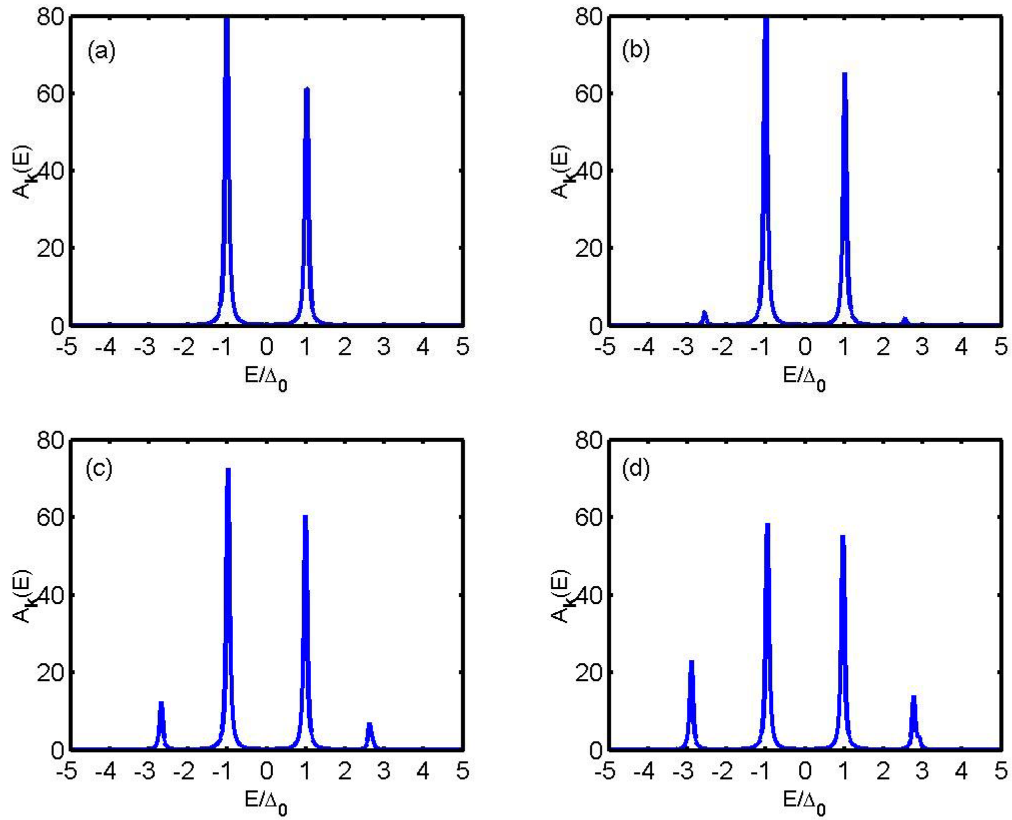
Ansatz for mode:

$$\chi(\mathbf{q}; i\Omega_l) = -\frac{N\delta_{\mathbf{q},\mathbf{Q}}}{2}\left[\frac{1}{i\Omega_l - \Omega_0} - \frac{1}{i\Omega_l + \Omega_0}\right]$$

$\mathbf{Q} = (\pi, \pi)$ and $\Omega_0 = 0.15$.

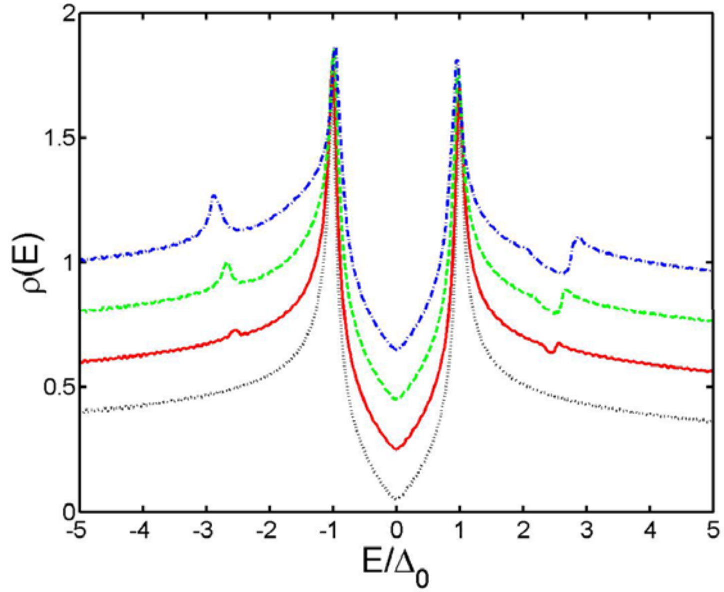
Spectral function at M point

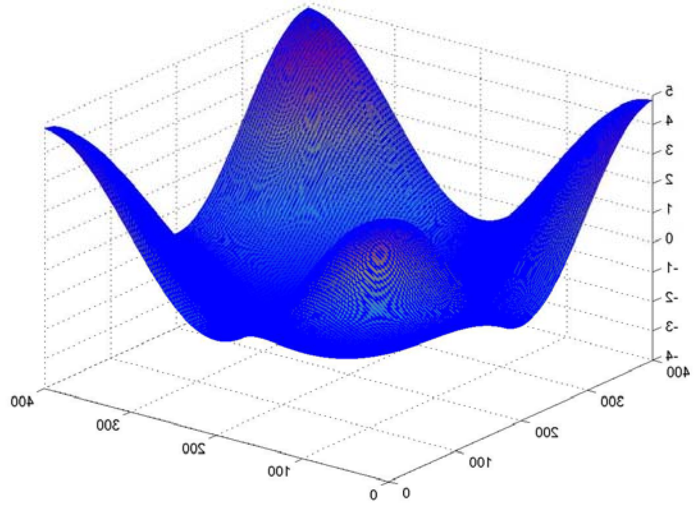




$$g/\Delta_0 = 0, 1, 2, 3$$

Band density of states



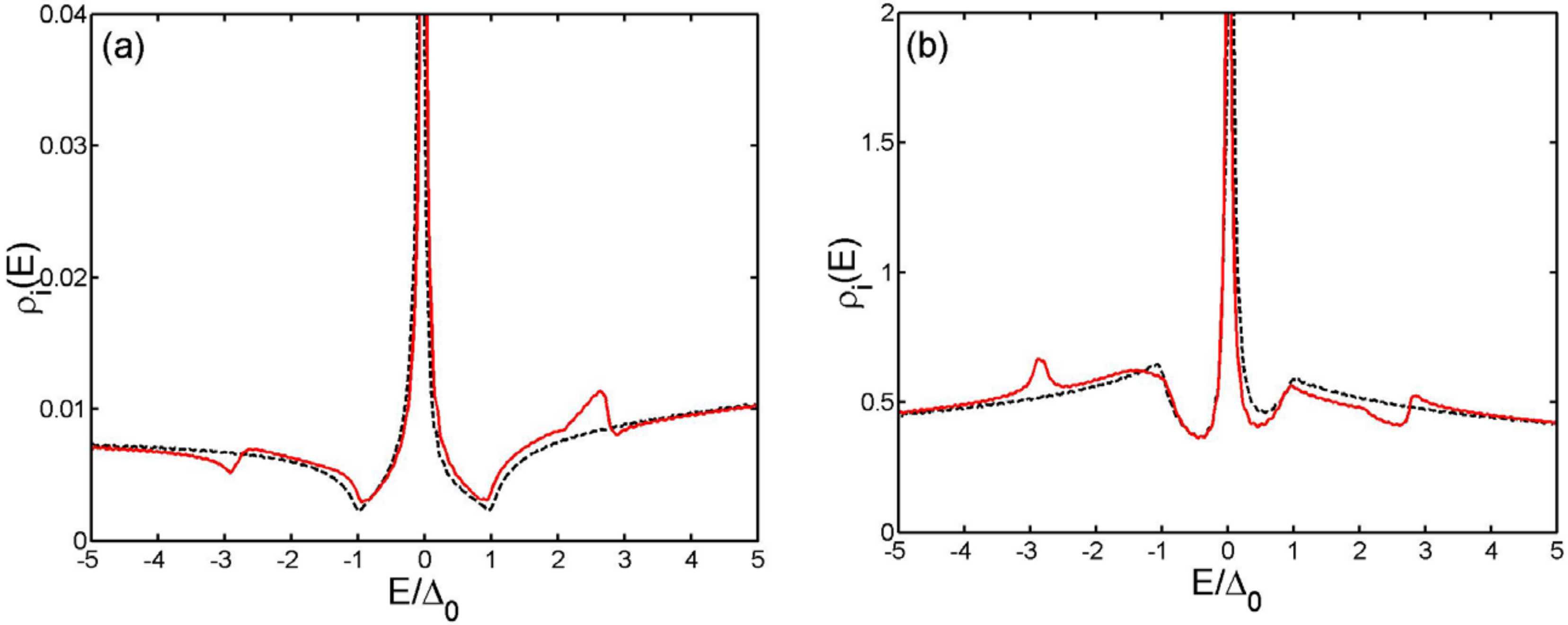


Translationally invariant image

$\varepsilon_{\mathbf{k}}$

Local density of states

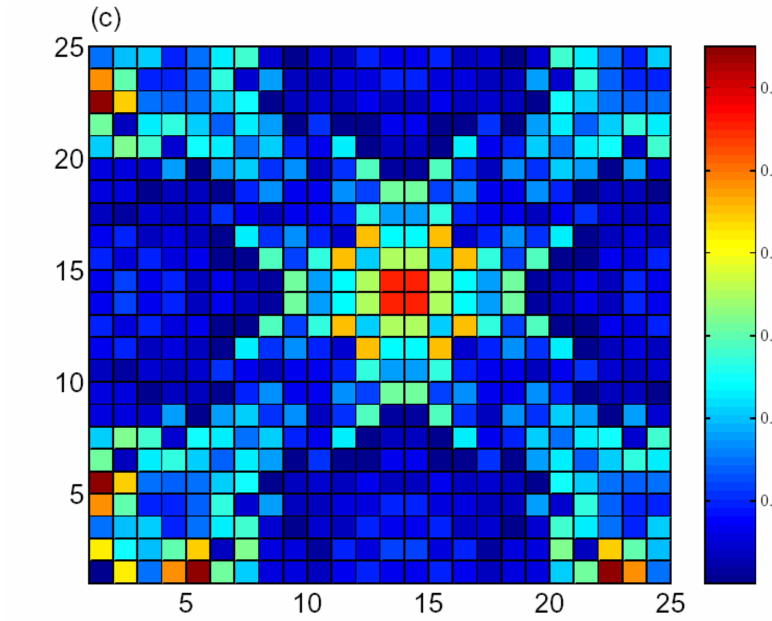
$$U_0 = 100\Delta_0 \quad g = 3\Delta_0$$

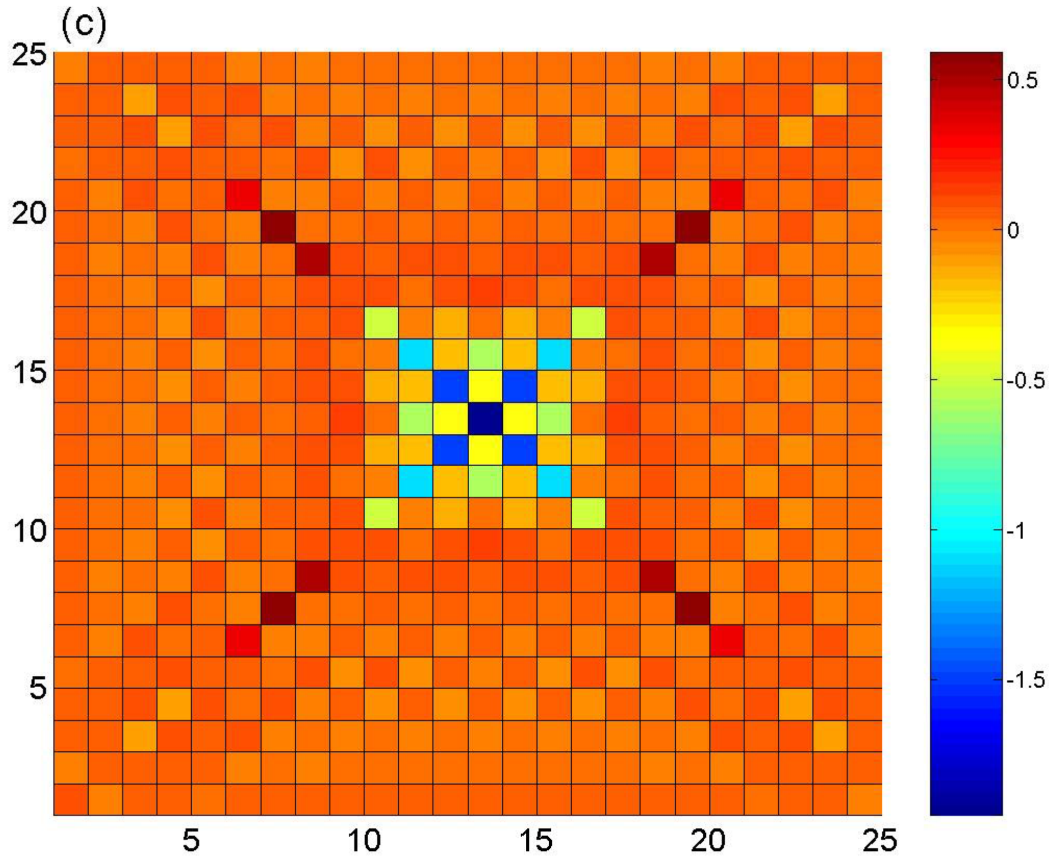


$$\mathbf{r}_i = (0,0) \qquad \mathbf{r}_i = (1,0)$$

LDOS imaging at $E=-E_1$ (Contrast)

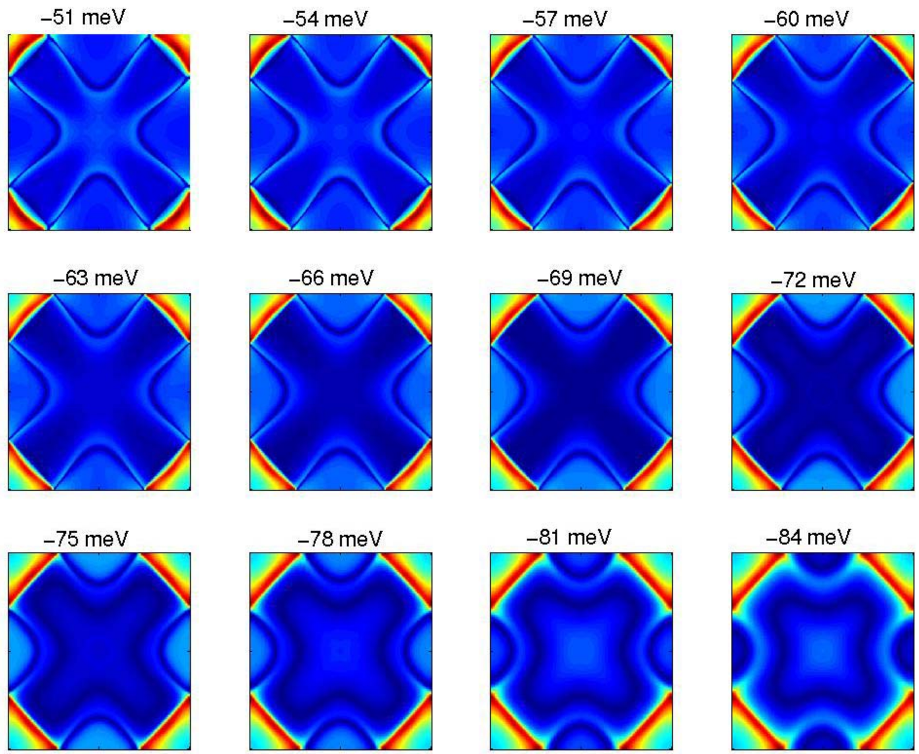
Scattering from the local center produces the modulation at Q





Novel collective mode spectroscopy (neutron or lattice)

Energy evolution of FT spectrum in the presence of B1g and half-stretching breathing collective modes --- 1



$$\omega_{B_{1g}} = 36 \text{ meV}$$
$$\omega_{br} = 72 \text{ meV}$$

$$\phi_x = \frac{-i}{\mathcal{N}_{\mathbf{k}}}[\xi_{\mathbf{k}} t_{x,\mathbf{k}} - t_{xy,\mathbf{k}} t_{y,\mathbf{k}}] \,,$$
$$\phi_y = \frac{i}{\mathcal{N}_{\mathbf{k}}}[\xi_{\mathbf{k}} t_{y,\mathbf{k}} - t_{xy,\mathbf{k}} t_{x,\mathbf{k}}] \,,$$
$$\phi_b = \frac{1}{\mathcal{N}_{\mathbf{k}}}[\xi_{\mathbf{k}}^2 - t_{xy,\mathbf{k}}^2] \,,$$

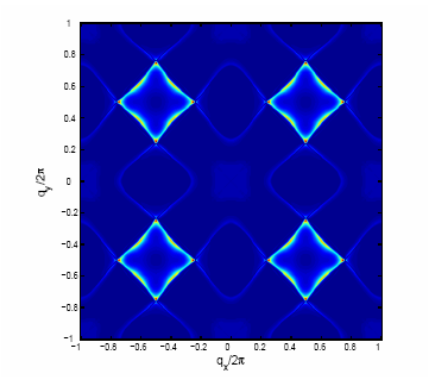
$$\mathcal{H}_{el-ph} = \frac{1}{\sqrt{N_L}} \sum_{\substack{\mathbf{k},\mathbf{q} \\ \sigma,\nu}} g_\nu(\mathbf{k},\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k}\sigma} (b_{\nu\mathbf{q}} + b^\dagger_{\nu,-\mathbf{q}})$$

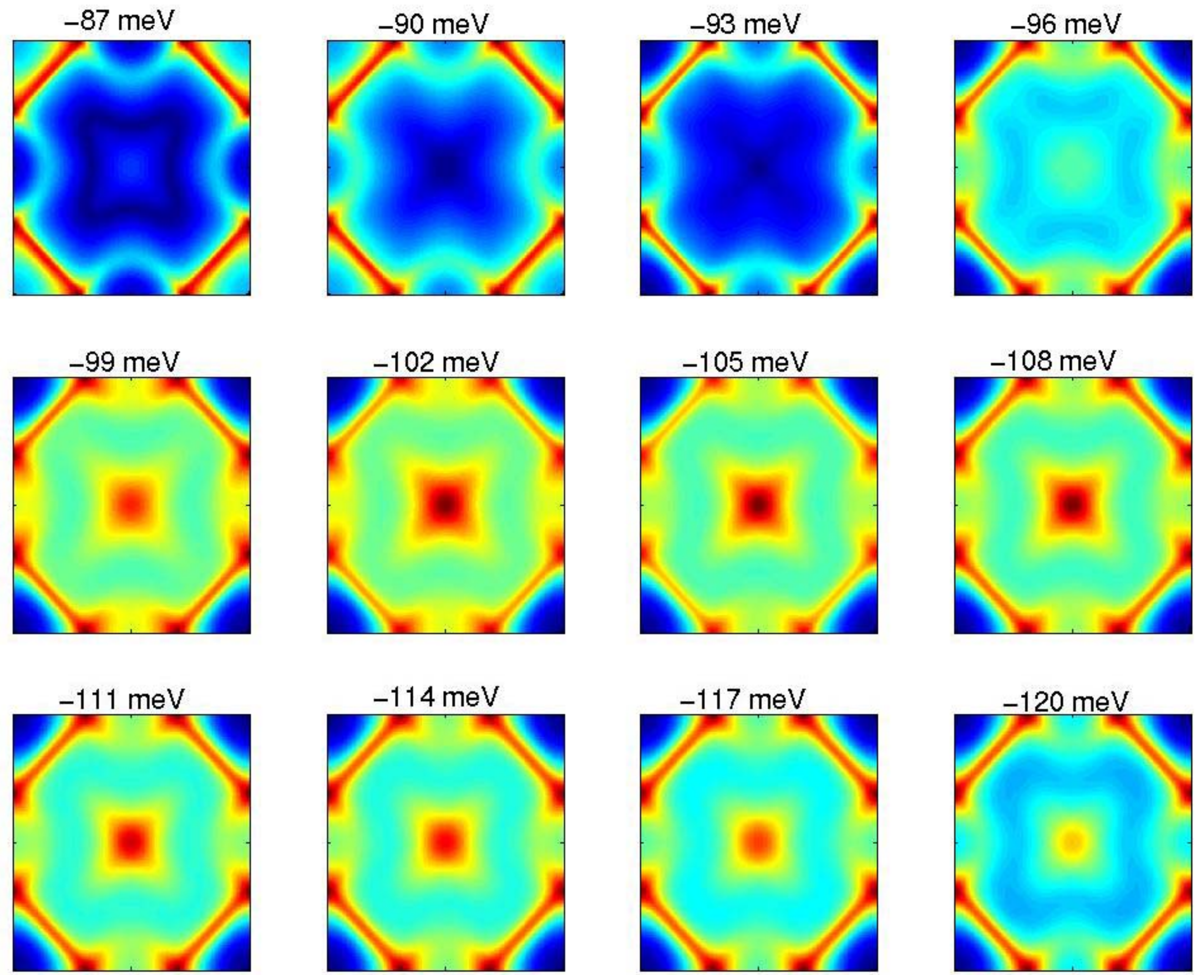
$$g_{B_{1g}}(\mathbf{k},\mathbf{q}) = \frac{g_{B_{1g},0}}{\sqrt{M(\mathbf{q})}} \{\phi_x(\mathbf{k})\phi_x(\mathbf{k}+\mathbf{q}) \cos(q_y/2) - \phi_y(\mathbf{k})\phi_y(\mathbf{k}+\mathbf{q}) \cos(q_x/2)\} \,,$$
$$g_{br}(\mathbf{k},\mathbf{q}) = g_{br,0} \sum_{\alpha=x,y} \{\phi_b(\mathbf{k}+\mathbf{q})\phi_\alpha(\mathbf{k}) \cos[(k_\alpha + q_\alpha)/2] - \phi_b(\mathbf{k})\phi_\alpha(\mathbf{k}+\mathbf{q}) \cos(k_\alpha/2)\} \,.$$

Energy evolution of FT spectrum in the presence of B1g and half-stretching breathing collective modes --- 2

n

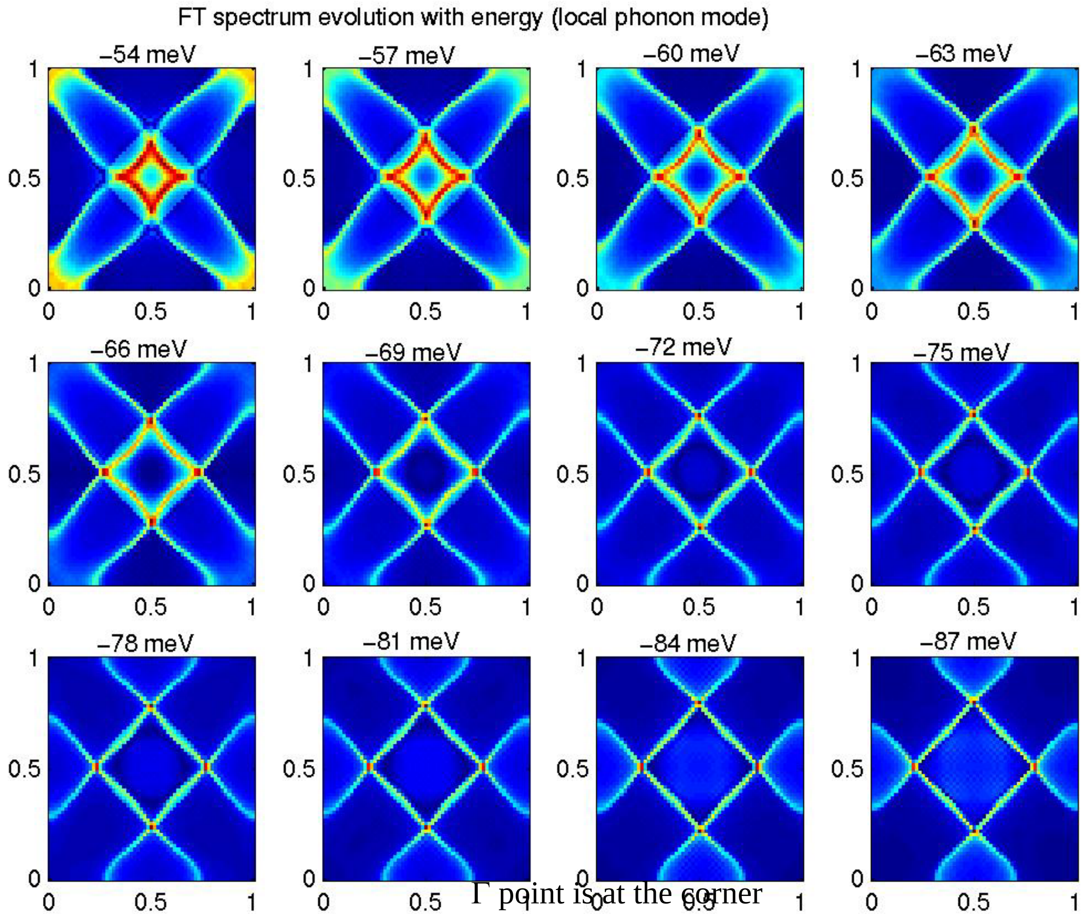
No filter!





Energy evolution of FT spectrum in the presence of a local phonon mode

No filter!



Γ point is at the corner

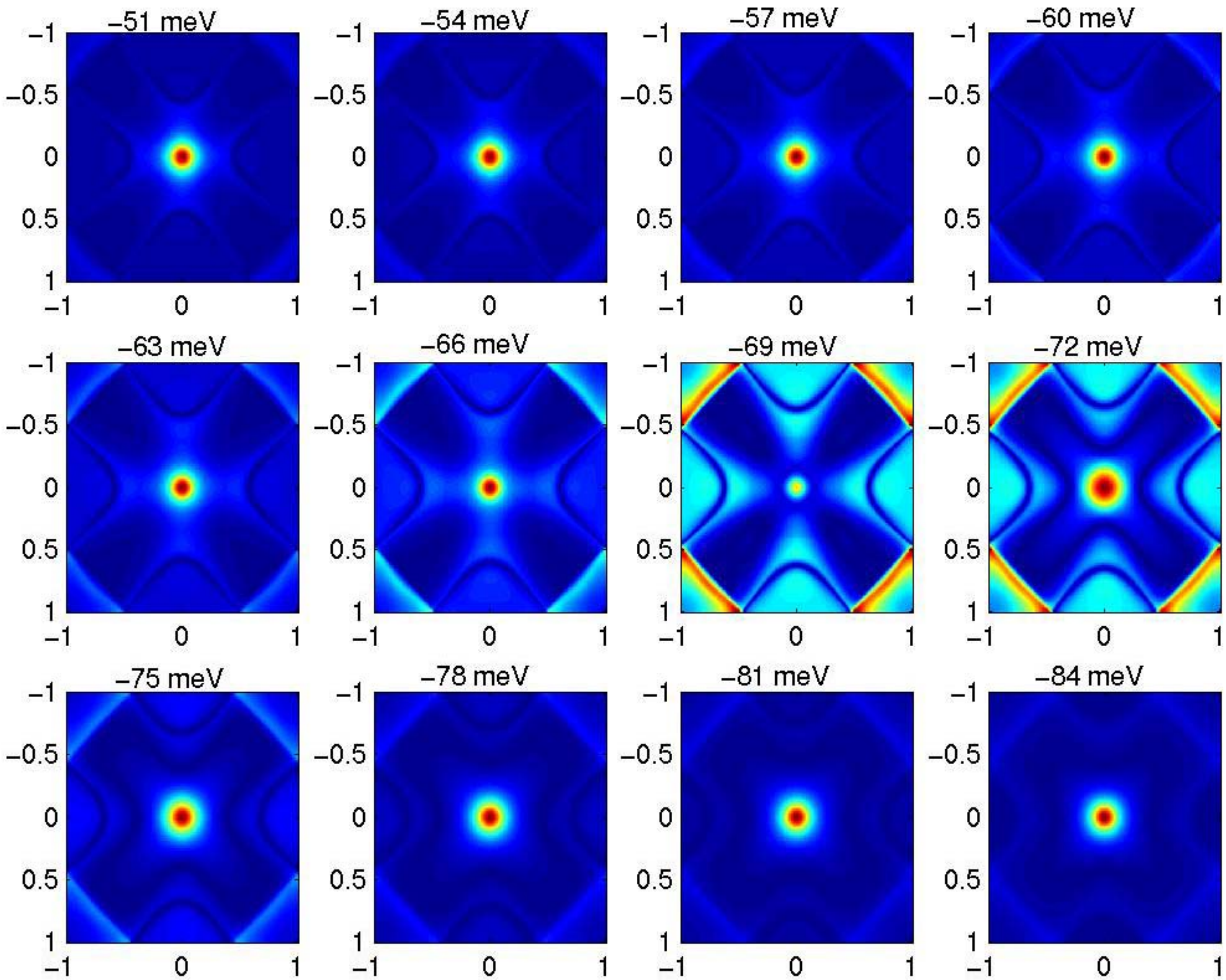
Note: k , k are in units of 2π/a

$$\mathcal{H}_{el-localph} = g_0 \sum_\sigma c^\dagger_{0\sigma} c_{0\sigma} (b_0 + b^\dagger_0)$$

$$\Omega_0 = 36 \text{ meV}$$

Energy evolution of FT spectrum in the present of B1g and half-stretched breathing collective modes --- 1

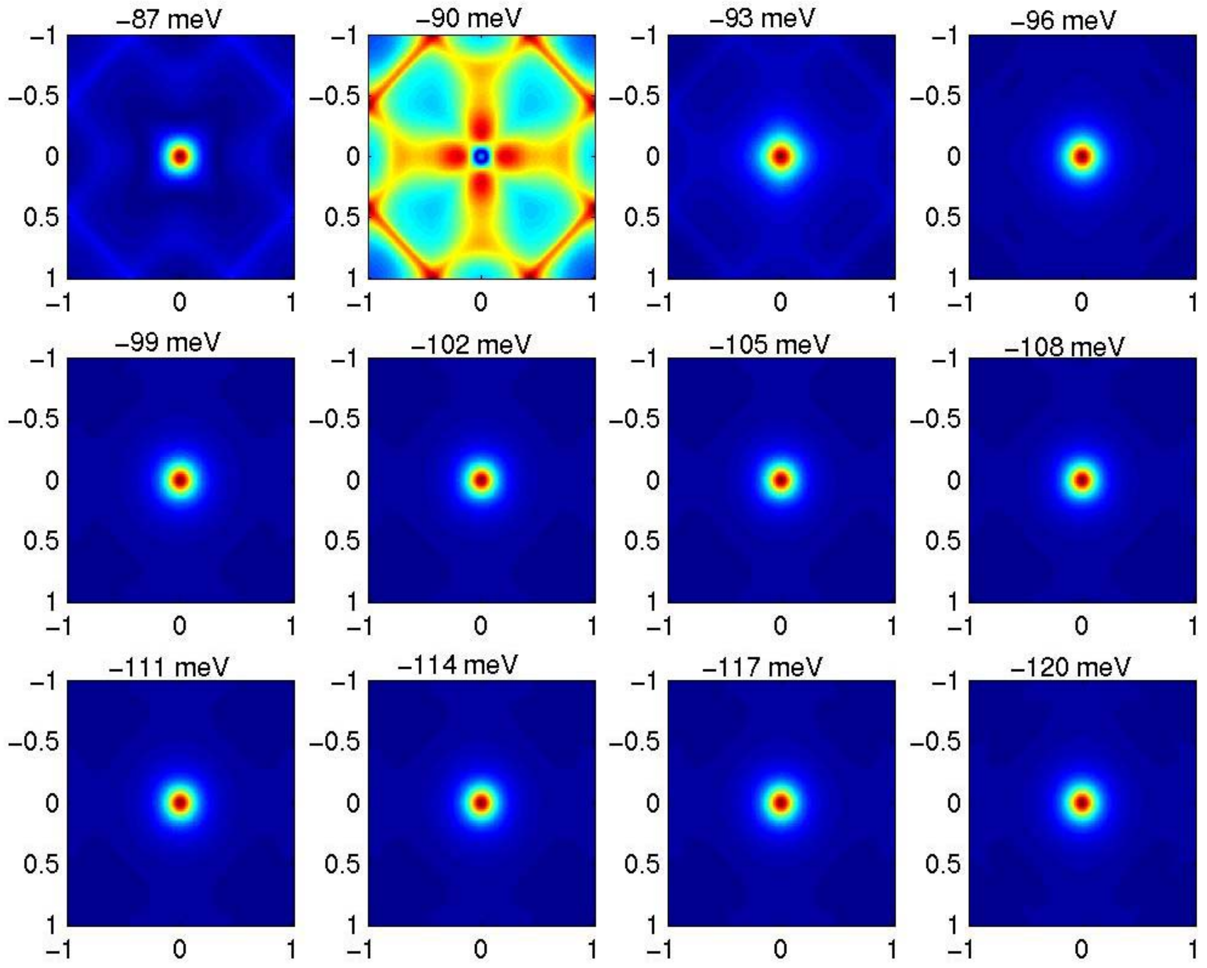
$$\text{Filter: } U(\mathbf{q}) = \frac{1}{1+r_c(\sin^2\frac{qx}{2}+\sin^2\frac{qy}{2})}$$



Note: k_x,k_y are in units of π/a. Γ point is located at the center

Energy evolution of FT spectrum in the presence of B1g and half-stretched breathing collective modes --- 2

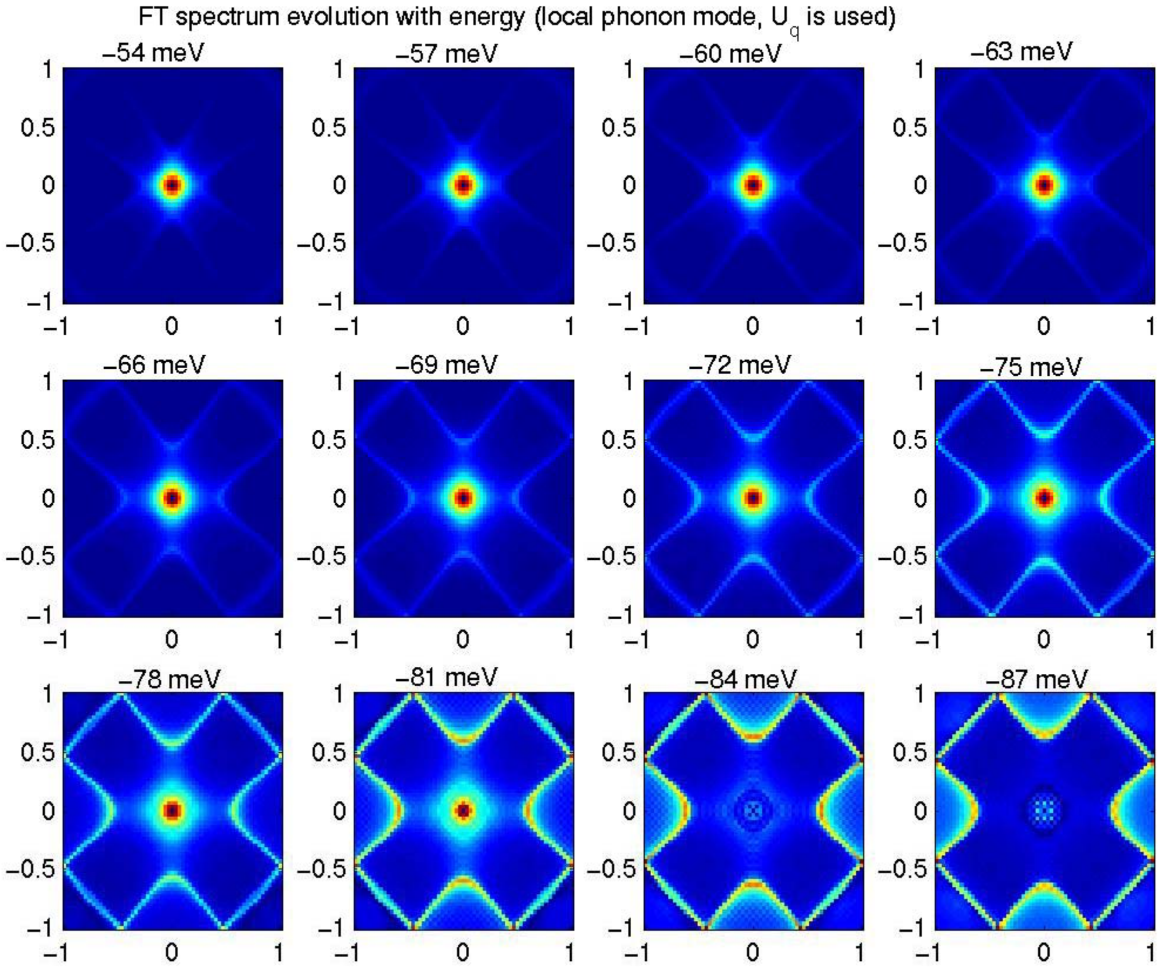
$$\text{Filter: } U(\mathbf{q}) = \frac{1}{1+r_c(\sin^2\frac{qx}{2}+\sin^2\frac{qy}{2})}$$



Note k_x, k_y are in units of π/a. Γ point is at the center

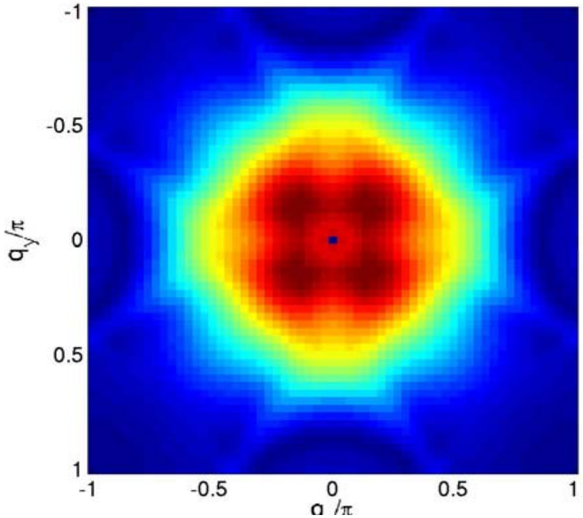
Energy evolution of FT spectrum in the presence of a local phonon mode

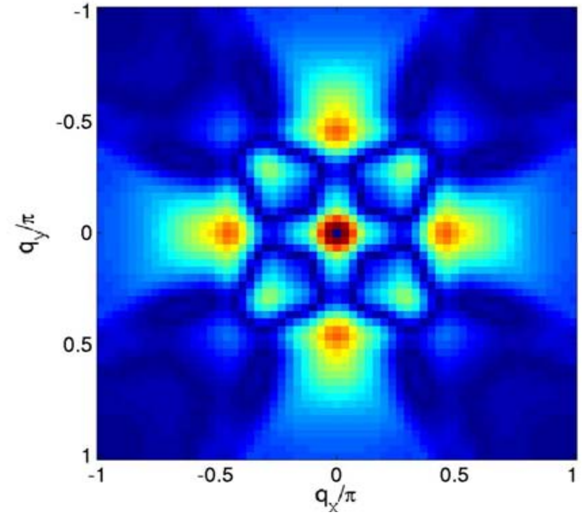
$$\text{Filter: } U(\mathbf{q}) = \frac{1}{1+r_c(\sin^2\frac{q_x}{2}+\sin^2\frac{q_y}{2})}$$

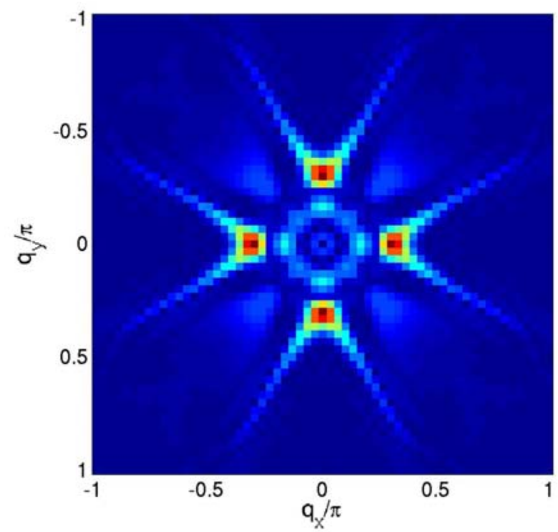


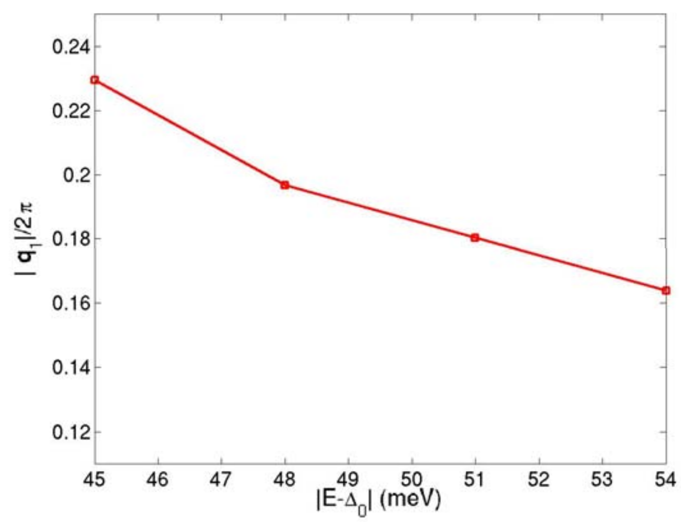
Note: K_x, k_y are in units of π/a, Γ point is at the center

Tau 1 FT IETS signals strong coupling self consistent calc

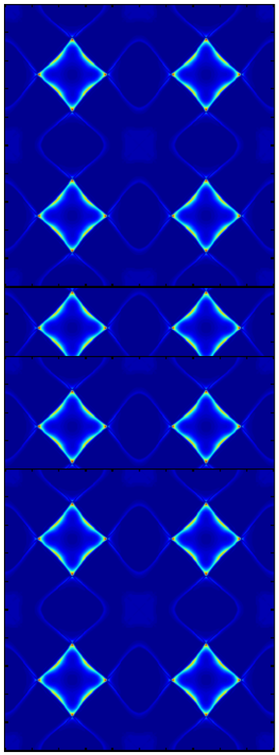








Experimental Algorithm



Measure a set of second-derivative images: $\frac{d^2 I}{dV^2}(\vec{r}, eV)$

Fourier transform: second-derivative images: $\frac{d^2 I}{dV^2}(q, eV)$

Identify energies: $\Omega = eV - \Delta$

and q –vectors:

of peaks in d2I/dV2 caused by $\vec{\vec{q}}(\Omega)$

Inelastic electron-boson interactions

Electron phonon cpupling example

$$\mathcal{H}_{el-ph} = \frac{1}{\sqrt{N_L}} \sum_{\substack{\mathbf{k},\mathbf{q}\\ \sigma}} g_\nu(\mathbf{k},\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k}\sigma} A_{\nu,\mathbf{q}} \,,$$

$$g_{B_{1g}}(\mathbf{k},\mathbf{q}) = \frac{g_0}{\sqrt{M(\mathbf{q})}} \{\phi_x(\mathbf{k})\phi_x(\mathbf{k}+\mathbf{q})\cos(q_y/2) - \phi_y(\mathbf{k})\phi_y(\mathbf{k}+\mathbf{q})\cos(q_x/2)\} \,,$$

$$g_{br}(\mathbf{k},\mathbf{q}) = g_0 \sum_{\alpha=x,y} \{\phi_b(\mathbf{k}+\mathbf{q})\phi_\alpha(\mathbf{k})\cos[(k_\alpha+q_\alpha)/2] - \phi_b(\mathbf{k})\phi_\alpha(\mathbf{k}+\mathbf{q})\cos(k_\alpha/2)\} \,,$$

$$\mathcal{D}_\nu(\mathbf{q};i\Omega_m) = \frac{1}{2}\left[\frac{1}{i\Omega_m - \Omega_\nu} - \frac{1}{i\Omega_m + \Omega_\nu}\right] \,,$$

$$\hat{\Sigma}(\mathbf{k};i\omega_n) = -\frac{T}{N_L} \sum_{\mathbf{q},\nu} \sum_{\Omega_m} g_\nu(\mathbf{k}-\mathbf{q},\mathbf{q}) g_\nu(\mathbf{k},-\mathbf{q}) \times \mathcal{D}_\nu(\mathbf{q};i\Omega_m)\hat{\tau}_3 \hat{\mathcal{G}}_0(\mathbf{k}-\mathbf{q};i\omega_n - i\Omega_m)\hat{\tau}_3$$