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

**Motivation:**

- Spectroscopy technique
- Properties of electron-boson interaction at nanoscale in real-space: local/delocalized?
- For anisotropic electron-boson interaction, measure directly momentum transfer and energy $\Omega_0$
- Ideally find the anisotropic electron-boson spectral density

**Collaborators:**

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Old results

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 voltage for three Al–Al oxide–Pb junctions taken at

$$H_t = c_e^T c_R T(x) + h.c.$$  
$$T(x) = t_0 (1 + \alpha x)$$

$x$ — 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
• $H_i = gc_\sigma(r=0)c_\sigma(r=0)x$

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

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

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

\[ \delta N(r, \omega) \sim g^2 (\omega - \Omega_0)^\gamma \Theta(\omega - \Omega_0) \]

where \( \gamma \) is the DOS power

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

\[ H = \sum_k c^\dagger_{k\sigma} \epsilon(k)c_{k\sigma} + \sum_k (\Delta(k)c^\dagger_{k\uparrow}c_{-k\downarrow} + h.c.) + \sum_{k,k',\sigma,\sigma'} JS \cdot c^\dagger_{k\sigma}\sigma\sigma'c_{k'\sigma'} + g\mu_B S \cdot B , \]

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

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

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

Previous Tunneling work

Correlation of Tunneling Spectra in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ 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$^5$


But no real-space or q-space information!
Model and formalism

\[ \mathcal{H} = \mathcal{H}_{BCS} + \mathcal{H}_{cp} + \mathcal{H}_{imp} \]

\[ \mathcal{H}_{BCS} = \sum_{k,\sigma} (\varepsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + \sum_k (\Delta_k c_{-k\downarrow}^\dagger c_{k\uparrow}^\dagger + \Delta_k^* c_{k\uparrow} c_{-k\downarrow}) \]

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

\[ \mathcal{H}_{imp} = U_0 \sum_\sigma c_{0\sigma}^\dagger c_{0\sigma} \]
Bare GF: $\hat{G}_0^{-1}(k; i\omega_n) = \begin{pmatrix} i\omega_n - \xi_k & \Delta_k \\ \Delta_k & i\omega_n + \xi_k \end{pmatrix}$.

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

Dressed GF: $\hat{G}_0^{-1}(k; i\omega_n) = \begin{pmatrix} i\omega_n - \xi_k - \Sigma_{11} & \Delta_k - \Sigma_{12} \\ \Delta_k - \Sigma_{21} & i\omega_n + \xi_k - \Sigma_{22} \end{pmatrix}$.
Model and formalism (cont’d)

Site-dependent GF (TMA) w/ imp:

\[ \hat{G}(i, j; E) = \hat{G}_0(i, j; E) + \hat{G}_0(i, 0; E) \hat{T}(E) \hat{G}_0(0, j; E) \]

\[ \hat{T}^{-1} = U_0^{-1} \sigma_3 - \hat{g}_0, \quad \hat{g}_0(i \omega_n) = \hat{G}_0(i, i; i \omega_n) \]

LDOS: \[ \rho_i(E) = -\frac{2}{\pi} \text{Im} G_{11}(i, i; E + i \gamma) \cdot \]

Band DOS \((U_0 = 0)\): \[ \rho(E) = \sum_k A_k(E). \quad A_k(E) = -\frac{2}{\pi} \text{Im} G_{0,11}(k; E + i \gamma). \]
Numerical results and discussions

Parameter values: \( t = 1.0, \ t' = -0.2 \ [\varepsilon_k = -2t(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y] \)

\( \Delta_0 = 0.1 \ [\Delta_k = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)] \)

Ansatz for mode:
\( \chi(q; i\Omega_l) = -\frac{\sqrt{N}}{2} \delta_{q,Q} \left[ \frac{1}{i\Omega_l-\Omega_0} - \frac{1}{i\Omega_l+\Omega_0} \right] \)
where \( Q = (\pi, \pi) \) and \( \Omega_0 = 0.15 \).
Spectral function at M point

\[ \frac{g}{\Delta_0} = 0, 1, 2, 3 \]
Band density of states

Translationally invariant image
Local density of states

\[ U_0 = 100 \Delta_0 \quad g = 3 \Delta_0 \]

\( \mathbf{r}_i = (0, 0) \)

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

\[ \omega_{B1g} = 36 \text{ meV} \]
\[ \omega_{br} = 72 \text{ meV} \]

\[ \phi_x = \frac{-i}{N_k} [\xi_k t_{x,k} - t_{xy,k} t_{y,k}] \]
\[ \phi_y = \frac{i}{N_k} [\xi_k t_{y,k} - t_{xy,k} t_{x,k}] \]
\[ \phi_b = \frac{1}{N_k} [\xi_k^2 - t_{xy,k}^2] \]

\[ \mathcal{H}_{cl-ph} = \frac{1}{\sqrt{N_L}} \sum_{\sigma,\nu} g_{\sigma,\nu} (k) a_{\sigma,\nu}^\dagger (k + q) a_{\sigma,\nu} (k - q) \]

\[ g_{B1g}(k, q) = \frac{g_{B1g,0}}{\sqrt{M(q)}} \{ \phi_x(k) \phi_x(k + q) \cos(q_y/2) - \phi_y(k) \phi_y(k + q) \cos(q_x/2) \} \]

\[ g_{br}(k, q) = g_{br,0} \sum_{\alpha=x,y} \{ \phi_{\alpha}(k + q) \phi_{\alpha}(k) \cos((k_\alpha + q_\alpha)/2) - \phi_{\alpha}(k) \phi_{\alpha}(k + q) \cos(k_\alpha/2) \} \]
Energy evolution of FT spectrum in the presence of B1g and half-stretching breathing collective modes --- 2

No filter!
Energy evolution of FT spectrum in the presence of a local phonon mode

\[ \mathcal{H}_{el-local ph} = g_0 \sum_\sigma c_\sigma^\dagger c_\sigma (b_0 + b_0^\dagger) \]

\[ \Omega_0 = 36 \text{ meV} \]
Energy evolution of FT spectrum in the present of B1g and half-stretched breathing collective modes --- 1

Filter: \( U(q) = \frac{1}{1 + r_c \left( \sin^2 \frac{q_x}{2} + \sin^2 \frac{q_y}{2} \right)} \)

Note: \( k_x, k_y \) are in units of \( \pi/a \). \( \Gamma \) point is located at the center.
Energy evolution of FT spectrum in the presence of B1g and half-stretched breathing collective modes --- 2

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

Note $k_x, k_y$ are in units of $\frac{\pi}{a}$. $\Gamma$ point is at the center
Energy evolution of FT spectrum in the presence of a local phonon mode

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

FT spectrum evolution with energy (local phonon mode, $U_q$ is used)

Note: $k_x, k_y$ are in units of $\pi/a$, $\Gamma$ 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 \( \frac{d^2 I}{dV^2} \) caused by \( \vec{q}(\Omega) \)

Inelastic electron-boson interactions
Electron phonon coupling example

\[ H_{el-ph} = \frac{1}{\sqrt{N_L}} \sum_{k, q} g_{\nu}(k, q) c_{k+q, \sigma}^\dagger c_{k, \sigma} A_{\nu, q}, \]

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

\[ g_{\delta r}(k, q) = g_0 \sum_{\alpha = z, y} \{ \phi_\beta(k + q) \phi_\alpha(k) \cos((k_\alpha + q_\alpha)/2) - \phi_\beta(k) \phi_\alpha(k + q) \cos(k_\alpha/2) \}, \]

\[ D_\nu(q; i\Omega_m) = \frac{1}{2} \left[ \frac{1}{i\Omega_m - \Omega_\nu} - \frac{1}{i\Omega_m + \Omega_\nu} \right], \]

\[ \hat{\Sigma}(k; i\omega_n) = -\frac{T}{N_L} \sum_{q, \nu} \sum_{\Omega_m} g_{\nu}(k - q, q) g_{\nu}(k, -q) \]
\[ \times D_\nu(q; i\Omega_m) \hat{\tau}_3 \hat{\tau}_0(k - q; i\omega_n - i\Omega_m) \hat{\tau}_3 \]