Effects of Pairing Potential Scattering on Fourier-Transformed Inelastic Tunneling Spectra of High-T_c Cuprate Superconductors with Bosonic Modes

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Recent scanning tunneling microscopy (STM) experimentally observed strong gap inhomogeneity in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO). We argue that disorder in the pair potential underlies the gap inhomogeneity, and investigate its role in the Fourier-transformed inelastic tunneling spectra as revealed in the STM. We find that the random pair potential induces unique **q**-space patterns in the local density of states (LDOS) of a d-wave superconductor. We consider the effects of electron coupling to various bosonic modes and find the pattern of LDOS modulation due to coupling to the B_{1g} phonon mode to be consistent with the one observed in the inelastic electron tunnneling STM experiment in BSCCO. These results suggest strong electron-lattice coupling as an essential part of the superconducting state in high-T_c materials.

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The extent to which collective excitations of high-T_c cuprates are manifested in their single-particle spectra is a long standing issue. The band renormalization effects, seen in the angle-resolved photoemission spectroscopy [1] (as well as in the break junction tunneling experiments [2]), have the characteristics of an electron-bosonic mode coupling. The "41 meV" spin resonance mode, a prominent feature in the spin excitation spectrum, is a natural candidate for electrons to couple to [3–5]. On the other hand, there are also phonon modes of similar energies. They may as well have the strongest influence on the single electron spectra [6–9]. At present, the issue remains controversial. Recently several of us proposed [10] a Fourier transform inelastic electron tunneling spectroscopy STM (FT-IETS STM) technique as a complimentary way to study the nature of the bosonic mode. The technique takes advantage of the pioneering work of the Fourier-transformed STM [11,12], and combines it with the vintage IETS [13–15]. Central to this technique is the Fourier transform of the energy derivative of tunneling conductance map in real space $d^2I/dV^2(\mathbf{r}, \text{eV}) \rightarrow d^2I/dV^2(\mathbf{q}, \text{eV})$. This **q**-space map, also called the Fourier map, contains information about inelastic scattering carriers off collective modes in the system. Theoretically, one finds peaks in **q** space and energy eV in this Fourier map of IETS that are related to the inelastic scattering off some collective excitations in the system.

Recently preliminary results from the first FT-IETS STM experiment has been reported in BSCCO [16]. One of the important observations of this work was that observed FT-IETS features' intensity near (π, π) is low. Instead, the strongest intensity appears at the wave vectors parallel to the Cu-O bond directions. These experimental results have in turn motivated us to compare the FT-IETS spectra near a potential scatterer in the cases of electrons coupled to the spin resonance and various phonon modes [17]. It was shown that all cases contain sharp features near (π, π), in disagreement with the experimental spectrum. This raises the question of whether the potential (τ_3) scattering alone correctly describes the impurities in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO), or the off-diagonal gap disorder is an important component of electronic inhomogeneity in these systems.

The ubiquitously observed nanoscale inhomogeneity in BSCCO presumably has its origin in the dopant atoms. This aspect has been investigated by studying the correlation between the gap inhomogeneity and the position of oxygen dopants [18]. It was shown that the local electronic states are not associated with charge density variations. To account for those features, Nunner *et al.* [19] proposed looking at the effect of random pairing potential fluctuations, the so-called τ_1 disorder. We adopt a similar approach and address the effect of τ_1 disorder on FT-IETS signatures.

We focus on the Fourier map of the energy derivative of the local density of states (LDOS), d^2I/dV^2, at $E \approx \pm(\Omega_0 + \Delta_0)$. Several typical bosonic modes are considered as possible scattering modes. We find that the results for τ_1 disorder model are qualitatively different from the case of potential disorder: (1) there are no strong signatures in the **q** space near (π, π) in any of the electron-boson couplings; (2) the highly anisotropic coupling of electrons to the out-of-plane out-of-phase oxygen buckling B_{1g} phonon mode gives rise to a Fourier pattern similar to the IETS-STM experiment in BSCCO [16]. Our results are also consistent with the in-plane breathing mode although the agreement with the data is not as good. This consistency with the experimentally observed IETS spectra is encouraging as it opens up a way to characterize the strong scattering features in IETS in terms of specific boson modes. Both ARPES and STM need this kind of input to adequately understand the contributions of different collective modes. This Letter represents a first step along this direction.

We start with a model Hamiltonian for a two-dimensional d-wave superconductor with the coupling of electrons to bosonic modes:

$$\mathcal{H} = \mathcal{H}_{\rm BCS} + \mathcal{H}_{\rm el\text{-}boson} + \mathcal{H}_{\rm imp}. \qquad (1)$$

Here the bare BCS Hamiltonian, $\mathcal{H}_{\rm BCS} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + \Delta^*_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow})$, where the normal state energy dispersion is given by [20], $\xi_{\mathbf{k}} = -2t_1(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y - 2t_3(\cos 2k_x + \cos 2k_y) - 4t_4(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) - 4t_5 \cos 2k_x \cos 2k_y - \mu$, with $t_1 = 1$, $t_2 = -0.2749$, $t_3 = 0.0872$, $t_4 = 0.0938$, $t_5 = -0.0857$, and $\mu = -0.8772$, and the d-wave gap dispersion $\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)$. Unless specified explicitly, the energy is measured in units of t_1 hereafter. The coupling of the electrons to bosonic modes is modeled by the Hamiltonian $\mathcal{H}_{\rm el\text{-}boson} = \frac{1}{\sqrt{N_L}} \sum_{\mathbf{k},\mathbf{q},\sigma} g_\nu(\mathbf{k},\mathbf{q}) \times c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k}\sigma}(b_{\nu\mathbf{q}} + b^\dagger_{\nu,-\mathbf{q}})$ for the buckling B_{1g} ($\nu = 1$) and the in-plane half-breathing ($\nu = 2$) modes, while $\mathcal{H}_{\rm el\text{-}boson} = \frac{g_0}{2N_L} \sum_{\mathbf{k},\mathbf{q},\sigma,\sigma'} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} (\mathbf{S}_{\mathbf{q}} \cdot \boldsymbol{\sigma}_{\sigma\sigma'}) c_{\mathbf{k},\sigma'}$ for the spin resonance mode. For the phonon modes, we consider the cases where the coupling matrix element is either highly anisotropic, dependent on both $\mathbf{k}$ and $\mathbf{q}$, or is only $\mathbf{q}$ dependent. In the following we use the notation B_{1g}-I and br-I for the former type of phonon modes while B_{1g}-II and br-II for the latter type. Detailed expression of the coupling matrix elements for these types of phonon modes can be found in Ref. [17]. The third term describes the quasiparticles scattered off a τ_1 impurity due to the inhomogeneity in pair potential rather than off a conventional τ_3 impurity. In the following, we consider a single τ_1 impurity in a *d-wave* superconductor. The resulting Fourier pattern should survive a white-noise random distribution of such τ_1 impurities in a realistic system. The impurity part of the Hamiltonian can then be written as

$$\mathcal{H}_{\rm imp} = \delta\Delta \sum_{\delta} \eta_\delta [c^\dagger_{0\uparrow} c^\dagger_{\delta\downarrow} + c^\dagger_{\delta\uparrow} c^\dagger_{0\downarrow} + \text{H.c.}], \qquad (2)$$

where $\eta_\delta = 1(-1)$ for $\delta = \hat{x}(\hat{y})$.

To be relevant to recent experimental realization, where no impurity-induced resonance state was observed, we assume the τ_1 impurity to have a weak scattering potential $\delta\Delta$. In this limit, we employ the Born approximation and arrive at the correction to the LDOS at the ith site, summed over two spin components:

$$\delta\rho(\mathbf{r}_i, E) = -\frac{2\delta\Delta}{\pi} \times \sum_{\delta} \eta_\delta \,\mathrm{Im}[\hat{\mathcal{G}}(i, 0; E + i\gamma)\hat{\tau}_1 \hat{\mathcal{G}}(\delta, i; E + i\gamma)]_{11}, \qquad (3)$$

where $\hat{\mathcal{G}}$ is the Green's function dressed with the bosonic renormalization effect and defined in the Nambu space [17]. From the perspective of the IETS, the energy derivative of the LDOS, $\frac{d\delta\rho(\mathbf{r}_i,E)}{dE}$, is the quantity we are most interested in. It corresponds to the derivative of the local differential tunneling conductance (i.e., d^2I/dV^2). The Fourier component of the differential LDOS is then given by $\frac{d\delta\rho(\mathbf{q},E)}{dE} = \sum_i \frac{d\delta\rho(\mathbf{r}_i,E)}{dE} e^{-i\mathbf{q}\cdot\mathbf{r}_i}$ with the spectral weight defined as $P(\mathbf{q}, E) = |\frac{d\delta\rho(\mathbf{q},E)}{dE}|$.

We consider here for comparison the coupling of electrons to spin resonance mode, B_{1g} and breathing phonon modes. For the numerical calculation, we take the superconducting energy gap $\Delta_0 = 0.1$, the frequency of all bosonic modes $\Omega_0 = 0.15$. The τ_1 impurity scattering strength $\delta\Delta$ is taken to be 50% of the superconducting energy gap. The coupling strength for all types of bosonic modes is calibrated to give at the Fermi energy $E = 0$ an identical frequency renormalization factor in the self energy. The same procedure as in Ref. [17] is followed to obtain the Fourier spectral weight $P(\mathbf{q}, E)$.

In Fig. 1, we present the results of the Fourier spectrum, $P(\mathbf{q}, E)$, at the energy $E = -(\Delta_0 + \Omega_0)$ for a d-wave superconductor with the electronic coupling to the bosonic modes. For comparison, the same spectrum is also shown (last panel) for the case of no mode coupling. Note that the case without the mode coupling, the energy Ω_0 has no special meaning in the context of the electronic properties, and the energy $E = -(\Delta_0 + \Omega_0)$ is chosen merely for comparison to the case of mode coupling. The energy $E = -(\Delta_0 + \Omega_0)$ corresponds to the position where the bosonic modes are excited, signaling a peak in the IETS d^2I/dV^2-V tunneling spectrum [17]. First of all, the Fourier map in each case does not display any peak structure at large $\mathbf{q}$ near $(\pm\pi, \pm\pi)$ and $(\pm\pi, \mp\pi)$ which appears persistently with the τ_3 scattering [17]. Instead the Fourier spectral weight is minimal in intensity (dark blue area in the figure) in these regions. The map for the case of electronic coupling to the B_{1g}-I phonon mode shows locally strongest intensity (red spots) at $\mathbf{q}$ about $(\pm\frac{2\pi}{4}, 0)$ and $(0, \pm\frac{2\pi}{4})$. The peak intensity at $\mathbf{q}$ near $(\pm\frac{2\pi}{4}, \pm\frac{2\pi}{4})$ and $(\pm\frac{2\pi}{4}, \mp\frac{2\pi}{4})$ is much weaker than those along the bond directions. The map for the case of the coupling to the br-I phonon mode exhibits locally strongest intensity (red spots) at $\mathbf{q}$ near $(\pm\frac{3\pi}{10}, 0)$ and $(0, \pm\frac{3\pi}{10})$. In addition, each of these red spots has a double-tail structure, which is absent in the case of B_{1g}-I mode coupling. The maps for the cases of the B_{1g}-II and spin resonance mode coupling exhibit similar $\mathbf{q}$ structure. The finite intensity is uniformly distributed on a circular strip near $|\mathbf{q}| = \frac{2\pi}{4}$ and becomes stronger as $\mathbf{q}$ approaches the zero point. No locally distinguishable strongest intensity peak can be identified at $\mathbf{q} = (\pm\frac{2\pi}{4}, 0)$ and $(0, \pm\frac{2\pi}{4})$. The map for the coupling to the br-II phonon mode exhibits locally the highest intensity (red spots) at $\mathbf{q}$ near $(\pm\frac{2\pi}{4}, \pm\frac{2\pi}{4})$ and $(\pm\frac{2\pi}{4}, \mp\frac{2\pi}{4})$. No peaks are found at $\mathbf{q}$ near $(\pm\frac{2\pi}{4}, 0)$ and $(0, \pm\frac{2\pi}{4})$. The map for

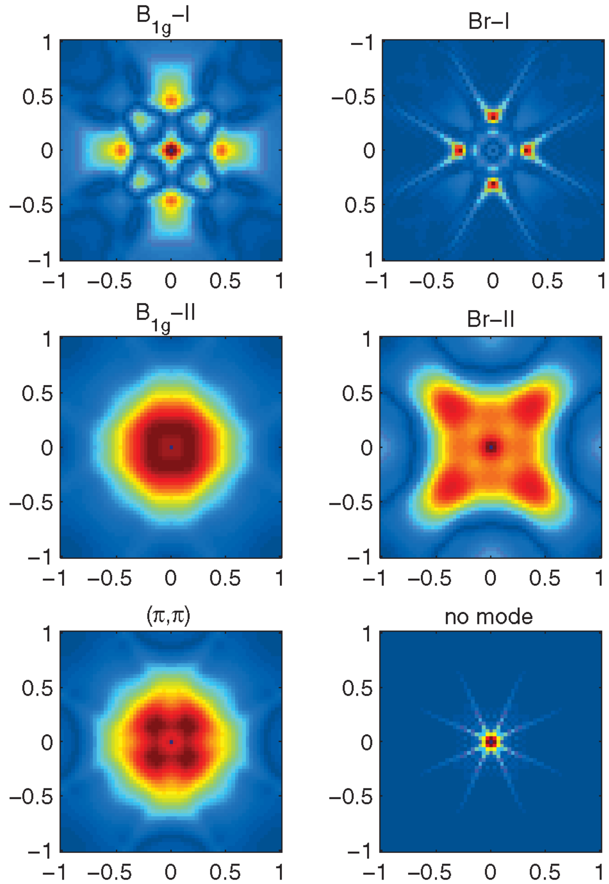

FIG. 1 (color). The Fourier spectrum of the energy derivative LDOS at the energy $E = -(\Delta_0 + \Omega_0)$ for a d-wave superconductor with the electronic coupling to the B_{1g}-I, br-I, B_{1g}-II, br-II, spin resonace modes. For comparison, the spectrum is also shown for the case of no mode coupling.

the case of no mode coupling shows an eight-tail star shape at $\mathbf{q} = (0, 0)$, which consists of the head-on overlap of four red spots, such as those appearing in the case of the br-I phonon mode coupling each with two tails. As we have already emphasized, experimentally, the Fourier map of d^2I/dV^2 shows intensity peaks only at $\mathbf{q} = (\pm\frac{2\pi}{5}, 0) \pm 15\%$ and $(0, \pm\frac{2\pi}{5}) \pm 15\%$ [16]. Therefore, by comparison with the experimental data, our new FT-IETS STM analysis also supports the notion [2–9] that the electronic band must be renormalized by its coupling to the bosonic modes. In particular, the results based on the scenario of highly anisotropic coupling of electrons to the B_{1g} phonon mode are in best agreement with the IETS-STM data in BSCCO.

In Fig. 2, we present the energy evolution Fourier pattern for the electronic coupling to the B_{1g}-I mode. It shows that the intensity peak structure along the bond direction is robust against the energy change. The characteristic q vector, at which the locally highest intensity is located, decreases slightly with the increased energy. This result is also not inconsistent with the preliminary experiment.

Our results demonstrate the important role the character of the scattering center plays in the Fourier spectrum. To explore this issue further, we note that, in the case of τ_1 scattering considered here, the Fourier spectrum can be expressed as follows,

$$\delta\rho(\mathbf{q}; E) = \frac{2\delta\Delta}{N_L}\sum_{\mathbf{k}}(\cos k_x - \cos k_y)\{[A(\mathbf{k}; E)K(\mathbf{k}+\mathbf{q}; E) + K(\mathbf{k}; E)A(\mathbf{k}+\mathbf{q}; E)] + [J(\mathbf{k}; E)B(\mathbf{k}+\mathbf{q}; E) + B(\mathbf{k}; E)J(\mathbf{k}+\mathbf{q}; E)]\}, \quad (4)$$

where

$$A(\mathbf{k}; E) = -\frac{2}{\pi}\,\mathrm{Im}[\mathcal{G}_{11}(\mathbf{k}; E + i\gamma)], \quad (5)$$

$$B(\mathbf{k}; E) = \mathrm{Re}[\mathcal{G}_{11}(\mathbf{k}; E + i\gamma)], \quad (6)$$

$$J(\mathbf{k}; E) = -\frac{2}{\pi}\,\mathrm{Im}[\mathcal{G}_{12}(\mathbf{k}; E + i\gamma)], \quad (7)$$

$$K(\mathbf{k}; E) = \mathrm{Re}[\mathcal{G}_{12}(\mathbf{k}; E + i\gamma)]. \quad (8)$$

This expression shows that, for the τ_1 scattering, the Fourier spectrum is determined by the $\mathbf{k}$ summation of the product terms constituting the imaginary (real) parts of the single-particle ($\mathcal{G}_{11}$) with the real (imaginary) parts of the anomalous ($\mathcal{G}_{12}$) Green's function in the superconducting state, weighted by a d-wave type form factor $\cos k_x - \cos k_y$. This scattering process with the τ_1 impurity is significantly different than the case of a τ_3 impurity scattering [17], where the convolution takes place between the real and imaginary parts of the same Green's function without the form factor. This difference of the scattering process matters significantly in the resulting Fourier map. As shown in Eq. (4), the form factor $\cos k_x - \cos k_y$ appearing in the τ_1 scattering case is identically zero along the diagonals in the first Brillouin, but reaches a maximum at the M points [$\mathbf{k} = (\pm\pi, 0)$ and $(0, \pm\pi)$] on the zone boundary. It then follows that any stronger intensity from

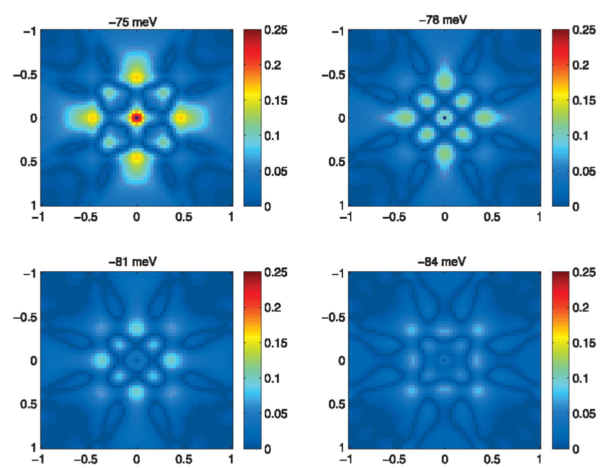

FIG. 2 (color). The Fourier spectrum of the derivative of the LDOS is shown at the various values of the energy for the case of the electronic coupling to the B_{1g}-I phonon mode. Here the energy has been measured by scaling $\Delta_0 = 30$ meV.

the product of AK, BJ connected by a $\mathbf{q}$ oriented close to the diagonals is strongly suppressed, while the intensity connected by $\mathbf{q}$ oriented parallel to the bond direction is enhanced. For the electronic coupling to the B_{1g}-I phonon mode, it has been found [17] that there is moderately strong intensity on the two split beams oriented perpendicular to the zone boundary at M points in the function A, B, J, and K. The form factor $\cos k_x - \cos k_y$ then tips the relative contribution from the product AK and BJ, giving rise to locally highest intensity at $\mathbf{q} = (\pm\frac{2\pi}{4}, 0)$ and $(0, \pm\frac{2\pi}{4})$ in the Fourier map (see the first panel of Fig. 1). These split beams of intensity are absent for the electronic coupling to other modes.

Our results naturally suggest additional means to further explore the electron-bosonic mode coupling experimentally. For instance, a Zn impurity acts as a nonmangetic potential center—a τ_3 scatterer. In this case, the sharp features near (π, π) should be observed in the FT-IETS spectrum. In the case of low-energy elastic scattering interference of quasiparticles, related effects have in fact been demonstrated. Indeed, strong signatures near $(\pm\pi, \pm\pi)$ and $(\pm\pi, \mp\pi)$ appear in the theoretical spectra near a τ_3 scatterer [21]. These features are not observed experimentally in the stoichiometrical BSCCO [11,12], but are seen around a nomagnetic Zn impurity in the doped BSCCO.

In conclusion, we have studied, for the first time, the τ_1-impurity-induced Fourier pattern of the energy derivative local density of states in a d-wave superconductor with the coupling of electrons to various bosonic modes. We consider B_{1g}, half-breathing, and spin (π, π) modes. Our results show that, at the mode energy shifted by the d-wave superconducting gap energy Δ_0, i.e., $E = \pm(\Delta_0 + \Omega_0)$, the coupling of electrons to the B_{1g} or breathing phonon modes, gives rise to a Fourier pattern similar to the preliminary Fourier-transformed IETS-STM experiment in BSCCO [16]. The coupling of electrons to the spin resonance mode, on the other hand, yields a Fourier spectrum that is inconsistent with the experiment. These results do not necessarily rule out the role of the spin-spin interactions as being relevant for superconductivity in BSCCO, instead they imply that electron-phonon coupling has a strong impact on the superconducting electronic structure. These results have important implications for our understanding of the electronic properties of the cuprates. They also demonstrate the potential of the FT-IETS STM technique, and highlight the importance of τ_1 scattering in the impurity-free BSCCO [19].

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