The effect of disorder on electronic Raman scattering in the superconducting state of iron pnictides

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Electronic Raman scattering measures a polarization-dependent scattering intensity which can provide information about the location of nodes in the energy gap of an unconventional superconductor as well as its overall symmetry. In this paper, we calculate the Raman intensity in the presence of disorder for several models of the iron pnictide superconducting state. We include, for completeness, d-wave and isotropic s± responses in addition to more realistic extended s± superconducting gaps. The effect of disorder is modeled using a self-consistent T-matrix approximation, and is studied in the limits of isotropic and intraband-only scattering. We show how recent experiments on Ba(Fe1−xCox)2As2 may be consistent with “node lifting” by intraband disorder.

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I. INTRODUCTION

Electronic Raman scattering is sensitive to low-lying excitations and can be performed for various polarizations of the incoming and outgoing photons. This polarization dependence preferentially samples different parts of the Brillouin zone, making Raman scattering an important tool with which to clarify the location of nodes and the symmetry of the gap in the superconducting state. Muschler et al.2 have recently performed Raman scattering measurements on single crystals of Ba(Fe1−xCox)2As2 (122) for two different concentrations of Co. The data demonstrate the existence of low energy quasiparticle excitations in the superconducting state. These quasiparticles could be a result of pairbreaking effects or due to the presence of nodes in the superconducting gap. In this paper we study the polarization dependent electronic Raman response in the presence of disorder in order to distinguish between these two possibilities.

Thus far, other experimental probes have not presented a convincing determination of a universal gap structure in the Fe-pnictides.3–4 This may be due to variations in sample quality and resolutions issues of different measurement techniques, but there is increasing speculation that these systems may possess a strong sensitivity of both the electronic structure and the pair state to small changes which affect electronic structure.5 This is because the Fermi surface consists of several nearly compensated electron and hole pockets, and because the pairing state is probably of an extended-s type which may possess “accidental” nodes or deep minima, i.e. structures depending on the details of the pairing interaction rather than the symmetry class. Nuclear magnetic resonance (NMR) studies6–9 showed a T1 spin lattice relaxation rate reminiscent of a gap with nodes. ARPES measurements on single crystals of 122-type materials10–15 measured the gap reporting isotropic or nearly isotropic gaps on all Fermi surface sheets. Penetration depth measurements16–21 have been fit both to an activated T-dependence, indicative of a fully gapped state, and low-T power laws, indicative of nodes in the superconducting gap. It is possible that these differences reflect genuinely different ground states in different materials due to intrinsic differences in the pairing, but it is important to disentangle these effects from those which arise from disorder, and in particular to distinguish between a disordered fully gapped state and a nodal state.

A popular candidate for the ground state of ferropnictides is the so-called s± state proposed by Mazin et al.22 In this state, found within a simple spin fluctuation model with strong interband scattering between nearly nested electron and hole pockets, the gap is isotropic on both electron and hole pockets but with a sign change between the two. Further theoretical work22–25 considered spin fluctuation pairing using band structures derived from tight binding fits to density functional theory results, and found s±-type states with highly anisotropic gaps, particularly on the electron sheets. We refer to this general class of states, which are in the same symmetry class as ordinary s-wave and isotropic s± states, as “extended-s” states here. These calculations also reported the near degeneracy of d-wave gaps in certain situations. The effect of nonmagnetic disorder on an s±, d-wave, and nodal extended-s is different and thus may help narrow the field of candidate superconducting gaps. In particular, it has been shown that for the accidental nodes of an extended s-wave state, intraband disorder can ‘lift’ the nodes, resulting in a fully-gapped state.26 On the other hand, if disorder is of the interband type, low-energy impurity midgap states can be created27–30 similar to Yu-Shiba states due to magnetic impurities in ordinary superconductors.

One complication is that changing the doping does not have the simple effect of creating more point-like disorder. To what extent a dopant is charged or magnetic, long or short ranged, and what changes it makes in band
structure upon doping requires careful study\textsuperscript{36,37} and is difficult to include consistently in a theory capable of calculating observable quantities. In the most naive approach, we will consider doping as loosely related to the concentration of scatterers in the sense that higher doping is a dirtier sample, with the caveat that effects on the electronic structure and pair interaction may also be present. Here we report the results of a calculation of the Raman intensity for $s_\pm$, $d$-wave, and experimentally inspired extended $s$-wave superconducting gaps, including disorder using a self-consistent T-matrix approximation (SCTMA). We show that for unitary scatterers, intraband scattering will average the gap and 'lift' the nodes of an extended $s$-wave state, leaving a fully developed gap for higher scattering rates due to disorder. When a strong interband scattering component is present, the creation of an impurity band competes with the tendency to lift the accidental gap nodes. In contrast to the extended-$s$ scenario, in an isotropic $s_\pm$ model, disorder causes the creation of low energy quasiparticles mimicking power law behavior of nodal states for some probes. One important difference between such a sign-changing isotropic state and a nodal extended-$s$ state, then, is that the addition of disorder fills in the gap as opposed to possibly creating it.

The form of the Raman spectrum will be influenced additionally by inelastic scattering processes. We expect these to be largely frozen out in the superconducting state at low energies, but they will be important for a proper treatment of the normal state spectrum and for energies near the maximum gap. Effects of this type will be treated elsewhere.\textsuperscript{28}

Our paper is organized as follows: in the first section we describe the theoretical background necessary to undertake this study. In the next section, we describe simple one and two band results for the $d$-wave and $s_\pm$ cases to help ground our understanding. Finally, we show the results from studying anisotropic $s$-wave states on all four Fermi sheets which we suggest captures all the essential qualitative features of the real Co-doped 122s.

II. THEORY OF ELECTRONIC RAMAN SCATTERING WITH DISORDER

Raman scattering is the inelastic scattering of polarized light from a material (for a review see Ref.\textsuperscript{1}). The cross section of the scattered light is proportional to

$$S_{\gamma\gamma} = \frac{\omega_{\text{scat}}}{\omega_{\text{inc}}} \frac{e^2}{mc^2} \left[1 + n_B(\omega)\right] \frac{I}{m} \int \chi_{\gamma\gamma}(\omega)$$

where

$$\chi_{\gamma\gamma}(\omega) = \int_0^\beta d\tau e^{-i\omega_\gamma \tau} \langle T_\gamma \hat{\rho}_\gamma(\tau) \hat{\rho}_\gamma(0) \rangle |_{i\omega_m \to w+i\delta},$$

and

$$\chi(q \to 0) = T \sum_n \sum_k Tr(e^{i\Omega_m}G(k, i\omega_n)\tau_3G(k, i\omega_n+i\Omega_m))$$

Here $\chi_{\gamma\gamma}$ is the Raman effective density-density correlation function for symmetry channel $\gamma$. The vertex, $\gamma_k$, accounts for the interaction of polarized light with charge density. The expression for the Raman effective density is $\rho = \sum_k \chi_k^\dagger \phi_{\gamma\sigma}^\dagger \phi_{\gamma\sigma}$. The full matrix Green’s function in the presence of scattering in the superconducting state is

$$G(k, \omega) = \frac{\tilde{\omega}_k \tau_0 + \tilde{\epsilon}_k \tau_3 + \tilde{\Delta}_k \tau_1}{\tilde{\omega}^2 - \tilde{\epsilon}_k^2 - \tilde{\Delta}_k^2},$$

where $\tilde{\omega} \equiv \omega - \Sigma_0$, $\tilde{\epsilon}_k \equiv \epsilon_k + \Sigma_3$, $\tilde{\Delta}_k \equiv \Delta_k + \Sigma_1$, and the $\Sigma_n$ are the components of the disorder self-energy proportional to the Pauli matrices $\tau_n$ in particle-hole (Nambu) space.

Generally, the vertex is determined by both density and current matrix elements between the conduction band and the excited states. However, in situations where one is interested in qualitative results like the present one, model Raman vertices classified by symmetry can be employed. For a crystal with $D_{4h}$ tetragonal symmetry, in-plane charge fluctuations transform according to the full symmetry of the lattice (irreducible representation $A_{1g}$), and do not change sign upon 90 degree rotation, or lower symmetry, as opposed to the $B_{1g}$ and $B_{2g}$ symmetry classes which change sign. Raman scattering probes long wavelength charge fluctuations. The $B_{1g}$ and $B_{2g}$ charge densities must average to zero within each unit cell, and are not coupled via the long-range Coulomb interaction. Thus the $B_{1g}$ and $B_{2g}$ Raman responses for a multi-band system consist of the sum of the contributions from each band. However, $A_{1g}$ fluctuations need not vanish over the unit cell, and therefore they can couple to isotropic charge density, giving rise the finite backflow. Therefore vertex corrections of both Coulomb and impurity type must be included in the $A_{1g}$ channel, which therefore becomes extremely difficult to treat consistently with disorder. We do not treat this polarization channel in this work. Finally, we neglect direct interband and resonant contributions to the Raman vertices. In this approximation, the vertex for Raman scattering measures the effective mass around the FS. We use the notation that $\vec{e}$ is a polarization vector.

$$\gamma_k = m \sum_{ab} e_a \frac{\partial^2 \phi}{\partial k_a \partial k_b} e_b$$

In a square lattice the $B_{1g}$ and $B_{2g}$ polarizations, the vertices can be expanded as:

$$B_{1g} : \gamma_k = \cos(k_x) - \cos(k_y)$$

and

$$B_{2g} : \gamma_k = \sin(k_x) \sin(k_y)$$

which along a circular Fermi surface become $\cos(2\theta)$ and $\sin(2\theta)$, respectively. It should be noted here that in the iron-pnictides use of the 1-Fe vs. the 2-Fe Brillouin zone will interchange $B_{1g}$ and $B_{2g}$ symmetries.
To include the effect of disorder we self-consistently solve for the self energies by including all scatterings off a single impurity and performing a disorder average. This is represented diagrammatically in Fig. 1. The T-matrix can be defined as

\[ G = G_0 + G_0 T G_0 + \cdots \]  

(2)

FIG. 1: Diagrams representing the self-consistent T-matrix approximation (SCTMA). The dashed lines are scattering off an impurity, and the single line is the self-consistent green’s function.

Using the Nambu notation, the single-particle self-energy in a superconductor can be decomposed as:

\[ \tilde{\Sigma}(k, \omega) = \sum_\alpha \Sigma_\alpha(k, \omega) \tilde{\tau}_\alpha, \]  

(3)

where \( \tilde{\tau}_\alpha \) are the Pauli matrices and \( \tilde{\tau}_0 \) is the unit matrix. Note that the band index is implicitly contained in the \( k \) index since we restrict pairing to individual Fermi surface sheets. Treating impurity-scattering in T-matrix approximation gives rise to the following self-energy

\[ \tilde{\Sigma}(k, \omega) = n_i \tilde{T}_{kk}(\omega), \]  

(4)

where \( n_i \) is the impurity concentration and \( T_{kk}(\omega) \) is the diagonal element of the T-matrix

\[ \tilde{T}_{kk}(\omega) = V_{kk'_{\gamma',\gamma}} \tilde{\tau}_3 + \sum_{k''} V_{kk'_{\gamma',\gamma}} \tilde{G}(k', \omega) \tilde{T}_{k'k''}(\omega). \]  

(5)

We define

\[ \Gamma = \frac{n_i n}{\pi N_0} \]

where \( n_i \) is the density of impurities, \( n \) of electrons, and \( N_0 \) the density of states at the Fermi level. For a constant potential, the case which we will consider in this paper, this expression becomes the series:

\[ \tilde{\Sigma}(\omega) = n_i V_0 \tilde{\tau}_3 \sum_n \left( \sum_{k'} G(k', \omega) V_0 \tilde{\tau}_3 \right)^n \]

Later we will restrict \( V_{kk''_{\gamma',\gamma}} \) to be constant for particular sets of momenta, either to allow transitions between all the Fermi sheets or to restrict transitions to remain within Fermi sheets.

The self-energy \( \tilde{\Sigma}(k, \omega) \) has to be solved self-consistently in combination with the single-particle Green’s function

\[ G(k, \omega)^{-1} = \tilde{G}_0(k, \omega)^{-1} - \tilde{\Sigma}(\omega). \]  

(6)

After solving for the self-energies, we insert them into the general expression for the Raman response. Beginning with a spectral representation:

\[ G(k, i\omega_n) = \int dx \left( \frac{-1}{\pi} \right) \frac{\text{Im} G(k, x)}{i\omega_n - x} \]

we arrive at a zero-temperature long-wavelength form,

\[ \text{Im} \chi_{\gamma,\gamma}(\Omega) = \sum_k \int_{-\Omega}^{0} dx \frac{1}{\pi} \gamma_k^2 T_r \left[ \text{Im} G(k, x) \tau_3 \text{Im} G(k, x +\Omega) \tau_3 \right]. \]

In terms of retarded and advanced Green’s functions, \( \text{Im} G = \frac{G^R - G^A}{2\pi} \):

\[ \text{Im} \chi_{\gamma,\gamma}(\Omega) = \frac{1}{4\pi} \langle N(\phi) \rangle \int d\xi \int_0^{\Omega} dx \]

\[ [F^{RR}(x - \Omega, x) - F^{RA}(x - \Omega, x)] + F^{AR}(x - \Omega, x) + F^{AA}(x - \Omega, x) \rangle. \]

where

\[ F^{a,b} = T_r [G^a(k, x - \Omega) \tau_3 G^b(k, x) \tau_3] \quad a, b = A, R \]

We have taken \( N(\phi) = N_0 \) in this paper. The angular brackets denote an average over the angle \( \phi \) around the Fermi surfaces.

We note here that for crossed polarizations selected \( B_{1g} \) and \( B_{2g} \) channels, the Raman response is additive for a many-sheeted Fermi surface. We also note that in the present approach we have neglected \( T_{\gamma\gamma} \) impurity vertex corrections for the Raman response. While for general momentum-dependent \( T_{\gamma\gamma} \), impurity vertex corrections are necessary for all channels, for momentum-independent scattering vertex corrections do not essentially modify the response for \( B_{1g} \) and \( B_{2g} \) polarizations\(^{39}\).

### III. RAMAN SCATTERING FOR DIRTY d-WAVE AND s\(_{\pm}\)-WAVE CASES

First we present results for \( d \)-wave and \( s_{\pm} \)-wave superconducting gaps. Early on, the \( s_{\pm} \) was proposed as a candidate for the gap structure in the iron-pnictides\(^{22}\). Indeed, for certain materials parameters, in particular the case where a Fermi surface pocket at \((\pi, \pi)\) appears, this state is crudely consistent with multiorbital spin-fluctuation calculations\(^{5,24,29}\). The qualitative features of the Raman response for such a state can be understood from a minimal two-Fermi-sheet model.

NMR and penetration depth measurements in some Fe-pnictide materials displayed power-law temperature dependences suggestive of nodes in a single band model\(^{25,21,22}\). The phenomenology was similar to what
FIG. 2: (Color online) Quasiparticle density of states $N(\omega)$ for isotropic $s_\pm$ state, normalized to normal state density of states $N_0$ vs. $\omega/\Delta_0$, where $\pm\Delta_0$ is the value of the gap on hole and electron sheets. $N_0$ is assumed constant on all Fermi sheets. Shown are various interband impurity scattering rates $\Gamma$ in units of $\Delta_0$.

FIG. 3: (Color online) Raman response $\text{Im} \chi(\omega)$ vs. $\omega/\Delta$ for both $B_{1g}$ and $B_{2g}$ polarizations for an $s_\pm$ state as in Fig. 2 for various interband impurity scattering rates $\Gamma$, in units of $\Delta_0$.

FIG. 4: (Color online) Density of states $N(\omega)/\Delta_0$ vs. energy $\omega/\Delta_0$ for a $d$-wave superconductor for various values of scattering rate $\Gamma/\Delta_0$ in unitarity limit.

was seen in cuprates, so it is useful to include a study of the $d$-wave case for comparison, to how the presence of a node in the superconducting gap manifests itself in the Raman response. The $d$-wave Raman response has been previously studied, for example in Refs. 40 39, and 43.

We first consider the $s_\pm$ state on two circular Fermi sheets, each with an isotropic constant gap in the superconducting state $\Delta_\pm = \pm\Delta_0$. The gaps differ by a minus sign, so inter-band scattering gives rise to pair-breaking and violates Anderson’s theorem. As we increase the scattering rate due to strong isotropic scatter-
ers, a low-energy impurity band is created in the density of states, show in Fig. 2. The clean Raman response simply reflects two clean $s$-wave gaps with a sharp gap edge at $2\Delta_0$. Note the line-shape in a fully gapped superconductor. This qualitative feature seems differs from a nodal superconductors’s line-shape, which still possesses a peak, only more symmetric about the center energy at $2\Delta_0$. One can understand the features in the Raman response as crudely similar to a convolution of the density of states with itself, so the effect of the impurity band on the Raman response is to create a nonzero threshold at $\omega < 2\Delta_0$, as shown in Fig. 3, corresponding to transitions between the impurity band and the gap edge. There is, in addition, a very small contribution from scattering within the impurity band itself at low energies (see insert Fig. 3).

In Figs. 4 and 5 we show the corresponding quantities calculated in the simple 1-band $d$-wave case, $\Delta(\theta) = \Delta_0 \cos(2\theta)$, as a canonical example of what one expects for a nodal unconventional superconductor. One fundamental difference with the $s_\pm$ case is the presence of low energy quasiparticles in the clean limit. The nodes in the superconducting gap allow for excitations in the low-energy density of states, shown in Fig. 4. Furthermore, the Raman polarization which weights the nodes ($B_{2g}$, in the $d$-wave case) yields differing power laws in $\omega$ from the polarization which vanishes along the nodal directions ($B_{1g}$), in contrast to the isotropic case where both of the Raman responses ($B_{1g}$ and $B_{2g}$) are the same. In the $d$-wave case, this is signaled by the presence ($B_{1g}$) or absence ($B_{2g}$) of a large peak at $2\Delta_0$. In both cases, increasing the scattering rate due to disorder increases the size of the impurity band, but the qualitative features of the $d$-wave Raman response, shown in Fig. 5 (a peak at $2\Delta_0$), excitations down to $\omega = 0$, differing response for differing polarizations) are unaltered by disorder. Beyond blurring of the sharp features, the effect of disorder
will change the low frequency behavior between from $\omega^2$ to $\omega$ in the $B_{1g}$ polarization for the $d$-wave case\textsuperscript{39}.

\section*{IV. RAMAN RESPONSE IN MODELS OF FERROPNICTIDES}

The full band structure of the Fe-pnictide LaOFeAs, determined by density functional calculations\textsuperscript{44,45}, can be accurately parameterized by a tight binding model with 5-bands\textsuperscript{24}. Generally, these materials have four Fermi surface sheets, shown in Fig. 6 in the “unfolded” or 1-Fe zone: two hole pockets around the gamma point and two electron pockets. The two Fermi surfaces about the gamma point are referred to as $\alpha$ sheets and the other two are $\beta$ sheets. The exact details of the band structure are sensitive to doping\textsuperscript{5}, and an additional hole pocket around the $(\pi, \pi)$ point can occur. We do not include the $(\pi, \pi)$-pocket because its effect is expected to stabilize isotropic gaps in the context of multiorbital spin-fluctuation calculations\textsuperscript{5,27-29}, and because it occurs (within a rigid band shift implementation of doping) for the hole-doped cases only. We focus here on electron doped materials on which experiments have been performed, which appear to show nodes or deep gap minima.

To model the $A_{1g}$, $B_{1g}$, and $B_{2g}$ polarizations measured in Muschler et al.\textsuperscript{2} the same choices were made for the extended s-wave gap on the $\alpha$ sheets (around the $\Gamma$ point) and $\beta$ sheets (around the M point) as in that paper:

$$\Delta_{\alpha_1}(\theta) = \Delta_0 \frac{1 + r \cos(4\theta)}{1 + r} \quad r = .75$$
$$\Delta_{\alpha_2}(\theta) = \Delta_0 \frac{1 - r \cos(4\theta)}{1 + r} \quad r = .75$$
$$\Delta_{\beta_1}(\theta) = -\Delta_0 \frac{1 - r \cos(2\theta)}{1 + r} \quad r = 1$$
$$\Delta_{\beta_2}(\theta) = -\Delta_0 \frac{1 + r \cos(2\theta)}{1 + r} \quad r = 1$$

The vertices for this state are chosen to be:

$$\alpha_1 \quad \gamma_{1g} = 0. \quad \gamma_{2g} = 0. \quad (11)$$
$$\alpha_2 \quad \gamma_{1g} = .25(-2) \sin(\theta) \cos(\theta) \quad \gamma_{2g} = .25 \cos(2\theta) \quad (12)$$
$$\beta_1 \quad \gamma_{1g} = .5(-2) \sin(\theta) \cos(\theta) \quad \gamma_{2g} = +1. \quad (13)$$
$$\beta_2 \quad \gamma_{1g} = .5(-2) \sin(\theta) \cos(\theta) \quad \gamma_{2g} = -1. \quad (14)$$

Note that the notation is now in the 2-Fe zone, for easy comparison with Ref. [2]. The vertices have been chosen to model experimental results with several constraints in mind. First, we must respect the underlying symmetry of the polarization state. In the $B_{1g}$ polarization, the response weighted is largely away from any Fermi sheet, which is reflected by a flat response in the model and data. The $B_{2g}$ polarization samples the electron ($\beta$) sheets\textsuperscript{2}. In the data and the model, there is a strong $T$-dependence to the data and a peak which appears below $T_c$, reflecting the corresponding gap function on these Fermi surfaces. More realistic calculations of the vertex functions $\gamma_k$ will be necessary for quantitative comparison with experiment.

Figure 7 shows the clean results for this model. In Muschler et al.\textsuperscript{2}, single crystals of Co doped Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ with $x = 0.061$ and 0.085 were studied. First, at $x=0.061$, the $B_{2g}$ spectra in the superconducting state are strikingly different from the $B_{1g}$ and
there are additional features at low energies due to the 
N of nodes leading to a characteristic that in the clean limit it has a marginal or “kissing” 2,41 Raman response V the potential for Co dopants in Ba-122 large density functional theory effective potential found in the density of states. The gap ∆ effect of increasing the intraband scattering rate on the spectra in the superconducting state. For this higher ∆1 behavior in the 2-Fe zone. Insert: low energy region.

The effect of disorder was calculated using the SCTMA in two limits: isotropic interband scattering for which V(⟨k,k′⟩) = V0, and intraband-only scattering for which V(⟨k,k′⟩) = 0 if k,k′ are on different Fermi sheets and V0 if k,k′ are on the same Fermi sheet. It was assumed that the potential V0 is large (unitarity limit), simulating the large density functional theory effective potential found for Co dopants in Ba-122.30 In Fig. we can see the effect of increasing the intraband scattering rate on the density of states. The gap ∆β,β(θ) has been chosen so that in the clean limit it has a marginal or “kissing” nodes leading to a characteristic ω^{1/2} behavior in the Raman response2,41, and the asymptotic low-ω behavior of N(ω) is indeed also ω^{1/2}, as seen in Fig. however there are additional features at low energies due to the small minimum gaps on the hole sheets. These features are largely suppressed in the clean Raman response, as shown in Fig. In the presence of intraband disorder, the nodes on the β sheets are lifted immediately, as seen in the density of states, creating a small but complete spectral gap Δ_{min}, as discussed in Mishra et al.30 This, in turn, is reflected with the creation of a gap in the Raman intensity in Fig. where there is a disorder induced gap edge in the response up to ω = 2Δ_{min}.

FIG. 7: (Color online) Clean B1g and B2g spectra for the model of the superconducting state defined in Eq. and in Eq. 10.

FIG. 8: (Color online) Density of states N(ω)/N0 for the extended s-wave state given in Eqs. Eq. 7-10 vs. ω/Δ0 for unitary intraband scattering rates Γ/Δ0. Insert shows low-energy behavior.

FIG. 9: (Color online) Raman intensity for the extended s-wave state given in Eqs. Eq. 7-10 vs. ω/Δ0 for various unitary intraband scattering rates Γ/Δ0 and polarization states B1g and B2g in the 2-Fe zone. Insert: low energy region.

The isotropic scatterers differ from the intra-band scatterers fundamentally in that inter-Fermi-sheet transitions allow for significant pair breaking, since the extended s-wave state changes average sign between electron and
hole Fermi surfaces. So in addition to the gap-averaging that occurs as we scatter from \( \mathbf{k} \) to \( \mathbf{k}' \), there is the additional effect of creating a low energy quasiparticles “impurity band.” This effect prevents the lifting of nodes, so while the gap becomes more isotropic, the impurity band is the most important low energy effect in the density of states. Indeed, as shown in Fig. 10, the DOS is reminiscent of the dirty \( s \)-wave case. There is also a striking similarity in the Raman intensity shown in Fig. 11 and the \( d \)-wave case. There are low energy quasiparticles all the way down to zero frequency, and we observe an enhancement of low frequency spectral weight.

**V. CONCLUSIONS**

Measurement of the Raman spectra in Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) revealed that at roughly 8% doping there is a gap in the response up to approximately 10 cm\(^{-1}\), in contrast to the 6% doped sample where there is a nonzero response down to zero frequency. This intriguing feature suggests a relation between cobalt doping, disorder, and the structure of the underlying superconducting gap. We have presented calculations of the Raman response as a function of frequency for varying scattering rates due to disorder in the self-consistent T matrix approximation. First, we demonstrated the differing effects of disorder on \( s_\pm \) and \( d \)-wave gaps to illustrate how a nodal superconductor contrasts with a sign-changing gapped state. The absence of low energy quasiparticles is an indication of a fully gapped state, but for systems with interband disorder scattering an impurity band is created which can mimic nodal behavior. We found, however, that in the presence of disorder the form of the main 2\( \Delta \) peak is largely unaffected; thus its observed symmetric form in the Muschler et al experiment is suggestive evidence for true nodal or near-nodal behavior.

More definitive information is provided by the Raman response at low energies. To study the anisotropic \( s \)-wave state in more detail, we have presented a set of model gap functions on the 2D Fermi surface sheets which capture the essential features of the experimental Raman response. It is immediately clear that for the dopings where measurements have been performed a nodal state is likely because of two factors: low frequency power law behavior of the Raman intensity down to zero energy, together with the very different responses for different polarizations. We then examined different kinds of disorder on such a state. A remarkable effect is the lifting of nodes by intraband scatterers for a highly anisotropic \( s \)-wave state, in rough agreement with the qualitative effect of gapping the Raman spectrum observed as the doping increased from 0.061 to 0.085 in Muschler et al. in Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\). The predicted effects of strong interband scattering at low energies were not observed, implying that the Co in this system acts primarily as an intraband scatterer\(^{28}\). Of course, the present calculations include only the effect of the impurity on pairbreaking, and neglect any direct effect on the pairing interaction, so direct conclusions may not be drawn.

This feature distinguishes nodal anisotropic \( s \)-wave states from isotropic \( s_\pm \) states in terms of how the response, and underlying superconducting gap, evolves with increasing disorder. It also is not possible in non-\( A_{1g} \) representations of the gap, like \( d \)-wave, because the nodes cannot be removed for lower symmetry superconducting gaps. We believe that these distinctions will provide a useful basis for the interpretation of Raman scattering experiments as doping or irradiation is tuned systematically in different samples.
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1. T.P. Devereaux, R. Hackl, Rev. Mod. Phys. 79, 175 (2007).
2. B. Muschler, W. Prestel, R. Hackl T.P. Devereaux J.G. Analytis, Jinn-Haw Chu, I.R. Fisher, Phys. Rev. B 80, 180510 (2009).
3. David C. Johnston arXiv:0805.4392 submitted to advances in physics
4. Johnpierre Paglione, Richard L. Greene arXiv:1006.4618
5. A. F. Kemper, T. A. Maier, S. Graser, H. Cheng, P. J. Hirschfeld, and D. J. Scalapino, to appear in New J. of Phys.
6. R. Klingeler, N. Leps, I. Hellmann, A. Carrington, N.D. K. Hashimoto, T. Shibauchi, T. Kato, K. Ikada, R. Wray, D. Qian, D. Hsieh, Y. Xia, L. Li, J.G. Checkelsky, K. Nakayama, T. Sato, P. Richard, A. Kreyssig, A. I. Goldman, J. Q. Yan, S. L. Bud’ko, F. C. Canfield, R. Prozorov, arXiv:0810.2295
7. H.-J. Grafe, D. Paar, G. Lang, N.J. Curro, G. Behr, J. Werner, J. Hamann-Borrero, C. Hess, N. Leps, R. Klingeler, and B. Buchner, arXiv:0808.0708
8. K. Ahilan, F.L. Ning, T. Imai, A.S. Sefat, R. Jin, A.M. McGuire, B.C. Sales, D. Mandrus, Phys. Rev. B 78, 100501(R) (2008).
9. T.Y. Nakai et al., J. Phys. Soc. Jpn. 77, 073701 (2008).
10. L. Zhao et al Chin. Phys. Lett. 25, 4402 (2008).
11. H. Ding, P. Richard, K. Nakayama, T. Sugawara, T. Arakane, Y. Sekiba, A. Takayama, S. Souma, T. Sato, T. Takahashi, Z. Wang, X. Dai, K. Fung, G.F. Chen, J.L. Luo, N.L. Wang, Europhys. Lett. 83, 47001 (2008).
12. T. Kondo, A.F. Santander-Syro, O. Copie, C. Liu, M.E. Tillman, E.D. Mun, J. Schmalian, S.L. Bud’ko, M.A. Tanatar, P.C. Canfield, A. Kaminski, Phys. Rev. Lett. 101, 047003 (2008).
13. D.V. Evtushinsky, D.S. Inosov, V.B. Zabolotnyy, A. Koitzsch, M. Knupfer, B. Buchner, G.L. Sun, V. Hinkov, A.V. Boris, C.T. Lin, B. Keimer, A. Varykhalov, A.A. Kordyuk, S.V. Borisenko, arXiv:0809.4455
14. K. Nakayama, T. Sato, P. Richard, Y.-M. Xu, Y. Sekiba, S. Souma, G. F. Chen, J.L. Luo, N.L. Wang, H. Ding, T. Takahashi, arXiv:0812.0063
15. L. Wray, D. Qian, D. Hsieh, Y. Xia, L. Li, J.G. Checkelsky, A. Pasupathy, K.K. Gomes, C.V. Parker, A.V. Fedorov, G.F. Chen, J.L. Luo, A. Yazdani, N.P. Ong, N.L. Wang, M.Z. Hasan, arXiv:0812.2061.
16. K. Hashimoto, T. Shibauchi, T. Kato, K. Ikada, R. Okazaki, H. Shishido, M. Ishikado, H. Kito, A. Iyo, H. Eisaki, S. Shamoto, and Y. Matsuda arXiv:0806.3149
17. L. Malone, J.D. Fletcher, A. Serafin, A. Carrington, N.D. Zhigadlo, Z. Bukowski, S. Katrych, and J. Karpinski, arXiv:0807.0876
18. C. Martin, R.T. Gordon, M. A. Tanatar, M. D. Vanmette, M. E. Tillman, E. D. Mun, P. C. Canfield, V. G. Kogan, G. D. Samolyuk, J. Schmalian, and R. Prozorov, arXiv:0807.0876
19. K. Hashimoto etal. arXiv:0810.3506
20. R. T. Gordon, N. Ni, C. Martin, M. A. Tanatar, M. D. Vannette, H. Kim, G. Samolyuk, J. Schmalian, S. Nandi, A. Kreyssig, A. I. Goldman, J. Q. Yan, S. L. Bud’ko, F. C. Canfield, R. Prozorov, arXiv:0810.2295
21. R. T. Gordon, C. Martin, H. Kim, N. Ni, M. A. Tanatar, J. Schmalian, L. I. Mazin, S. L. Bud’ko, P. C. Canfield, R. Prozorov, arXiv:0812.3683
22. J.D. Fletcher, A. Serafin, L. Malone, J. Analytis, J-H Chu, A.S. Erickson, I.R. Fisher, A. Carrington, arXiv:0812.3858
23. arXiv:0803.2740 Title: Unconventional sign-reversing superconductivity in LaFeAsO1-xFx Authors: I. I. Mazin, D.J. Singh, M.D. Johannes, M.H. Du Journal-ref: Phys. Rev. Lett. 101, 057003 (2008)
24. S. Graser, T. A. Maier, P. J. Hirschfeld, and D. J. Scalapino, New. J. Phys. 11 (2009)
25. A. V. Chubukov, D. V. Efremov, and I. Eremin, Phys. Rev. B 78, 134512 (2008).
26. K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki, Phys. Rev. Lett. 101, 087004 (2008).
27. K. Kuroki, H. Usui, S. Onari, R. Arita, and H. Aoki, Phys. Rev. B 79, 224511 (2009).
28. F. Wang, H. Zhai, Y. Ran, A. Vishwanath, and D. Lee, Physical Review Letters 102, 047005 (2009).
29. R. Thomale, C. Platt, J. Hu, C. Honerkamp, and B. A. Bernevig, Phys. Rev. B 80, 180505 (2009).
30. V. Mishra, G.R. Boyd, S. Graser, T. Maier, P.J. Hirschfeld, and D.J. Scalapino, Phys. Rev. B 79, 094512 (2009)
31. Yu, L., 1965, Acta Phys. Sin. 21, 75.
32. Shiba, H., 1968, Prog. Theor. Phys. 40, 435.
33. Hussey, N. Adv. Phys 51, 1685 (2002).
34. A.A. Golubov and I.I. Mazin, Phys. Rev. B 55, 15146 (1997).
35. Y. Senga and H. Kontani, arXiv:0809.0374.
36. arXiv:0812.2100 One of these is J. Phys. Soc. Jpn. 77, 113710 (2008).
37. A. Kemper, C. Cao, P.J. Hirschfeld, and H.-P. Cheng, Phys. Rev. B 80, 104511 (2009).
38. H. Wadati, I. Elfimov, G. A. Sawatzky, arXiv:1003.2663
39. A.F. Kemper, M. Korshunov, and P.J. Hirschfeld, to be published.
40. T.P. Devereaux and A.P. Kampf Int. J. Mod. Phys. B11, 2093 (1997).
41. T.P. Devereaux and D. Einzel, Phys. Rev. B 51, 163616357 (1995).
42. G.R. Boyd, T.P. Devereaux, P.J. Hirschfeld, V. Mishra, and D.J. Scalapino, Phys. Rev. B 79, 174521 (2009).
43. T. P. Devereaux, A. Virostek, A. Zawadowski Phys.Rev.B 54, 12537 (1996).
44. T. P. Devereaux Phys.Rev.Lett. 74, 4313 (1995)
45. D.J. Singh and M.-H. Du, Phys. Rev. Lett. 100, 237003 (2008).
46. C. Cao, P.J. Hirschfeld, H.-P. Cheng, Phys. Rev. B 77, 220506(R) (2008).