Resonance mode in B_{1g} Raman scattering: A way to distinguish between spin-fluctuation and phonon-mediated d-wave superconductivity

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We argue that Raman scattering in B_{1g} symmetry allows one to distinguish between phonon-mediated and magnetically mediated d-wave superconductivity. In spin-mediated superconductors, B_{1g} Raman intensity develops a resonance at a frequency $\Omega_{res}<2\Delta_{max}$, whose origin is similar to a neutron resonance. In phonon-mediated d-wave superconductors, such a resonance does not develop. Several extensions of the argument are presented.

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Does there exist an observable that would distinguish between magnetically mediated and phonon-mediated d-wave superconductivity? This question is motivated by the cuprates, for which recent measurements, particularly the observation of the kink in quasiparticle dispersion,[1] has revived the discussion as to whether the pairing in the cuprates is due to phonons rather than spin fluctuations. Both electron-phonon[2] and spin-fermion interactions[3] were advanced to explain the features in the quasiparticle dispersion. To truly distinguish between the two scenarios, one needs an observable for which they yield qualitatively different results.

We argue here that Raman scattering in B_{1g} symmetry is such a probe. We show that in spin mediated d-wave superconductors, the B_{1g} Raman intensity develops a resonance at a frequency $\Omega_{res}<2\Delta_{max}$, which does not occur in phonon-mediated d-wave superconductors. The resonance is similar to the excitonic resonance in the spin susceptibility of a d-wave superconductor.[4] The major difference is that the B_{1g} Raman resonance comes from fermions all around the Fermi surface and thus has a finite intrinsic width, whereas the resonance term in the spin susceptibility comes only from fermions in the antinodal regions and is a true bound state.

We first consider $S=1/2$ fermions interacting via a static potential $V^{pair}(k)$:

$$\mathcal{H}_{\rm int}=-\sum_{\mathbf{q},\mathbf{k},\mathbf{p}}\psi^{\dagger}_{\mathbf{k},\alpha}\psi^{\dagger}_{\mathbf{p}+\mathbf{q},\beta}V^{pair}_{\alpha\beta,\gamma\delta}(\mathbf{k}-\mathbf{p})\psi_{\mathbf{p}\gamma}\psi_{\mathbf{k}+\mathbf{q},\delta}. \qquad (1)$$

Here, summation over spin indices α,β,γ, and δ is understood. As the B_{1g} vertex has the same d-wave form as the pairing gap, we further approximate V^{pair} by its d-wave component $V^{pair}(\mathbf{k}-\mathbf{p})\propto d_k d_p$, where $d_k=[\cos(k_x a)-\cos(k_y a)]/2$. The gap is then $\Delta(\mathbf{k})=\Delta_0 d_k$.

The effective interaction $V^{pair}_{\alpha\beta,\gamma\delta}(\mathbf{k}-\mathbf{p})$ may be due to spin fluctuations or to phonons. For spin-mediated interaction, $V^{pair}_{\alpha\beta,\gamma\delta}(\mathbf{k}-\mathbf{p})=V_{spin}d_k d_p\boldsymbol{\sigma}_{\alpha\gamma}\cdot\boldsymbol{\sigma}_{\beta\delta}$, where $\boldsymbol{\sigma}$ are Pauli matrices. For phonon-mediated interaction, $V^{pair}_{\alpha\beta,\gamma\delta}(\mathbf{k}-\mathbf{p})=V_{ph}d_k d_p\delta_{\alpha\gamma}\delta_{\beta\delta}$. We will study the consequences for the Raman intensity. Our results also apply if phonons are replaced by charge density waves[5] or any other charge-induced pairing interaction.

If they both are to lead to an attraction in a d-wave channel, the signs of V_{spin} and V_{ph} must be different. Indeed, substituting effective interactions into the diagrammatic expression for the d-wave, spin-singlet pairing vertex $\psi^{\dagger}_{\mathbf{k},\alpha}\Phi_d(k)_{\alpha\beta}\psi^{\dagger}_{-\mathbf{k},\beta}$, where $\Phi_d(k)_{\alpha\beta}=\Phi d_k\sigma^y_{\alpha\beta}$, and using $\sigma^y_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\beta\delta}=\sigma^y_{\gamma\delta}$, $\sigma^y_{\alpha\beta}\boldsymbol{\sigma}_{\alpha\gamma}\cdot\boldsymbol{\sigma}_{\beta\delta}=-3\sigma^y_{\gamma\delta}$, we find that Φ is related to the bare vertex Φ_0 as

$$\Phi=\frac{\Phi_0}{1+3AV_{spin}};\quad \Phi=\frac{\Phi_0}{1-AV_{ph}} \qquad (2)$$

for spin-mediated or phonon-mediated interactions. $A\propto|\log\omega_c|$ is a conventional positive logarithmical factor. To obtain an attraction, one then needs V_{ph} to be positive, V_{spin} to be negative. This is the case when phonon-mediated interaction is peaked at small momenta Q, and spin-mediated interaction is peaked at Q near $(\pi/a,\pi/a)$.[2,6]

Let the system be a d-wave superconductor due either to phonons or spin fluctuations. The Raman vertex $\Gamma_{\alpha\beta}(k)$ in the B_{1g} channel has d-wave k dependence and is a spin scalar. We assume that $\Gamma_{\alpha\beta}(k)=\Gamma d_k\delta_{\alpha\beta}$. For a BCS superconductor without vertex or self-energy corrections, the B_{1g} Raman intensity $I_{B_{1g}}(\Omega)=\Gamma^2\chi''_0(\Omega)$, and $\chi''_0(\omega)$ is the imaginary part of the particle-hole bubble with two d-wave vertices (see, e.g., Ref. 7). In the normal state, $\chi_0(\Omega)$ vanishes, as there is no low-energy phase space available for scattering with $\mathbf{q}=0$. In the superconducting state, light scattering can break Cooper pairs with $\mathbf{q}=0$, and $\chi_0(\Omega)$ is given by Tsuneto function weighted with d_k^2.[7,8] The imaginary part of $\chi_0(\Omega)$ scales as Ω^3 at small Ω (Ref. 8) and diverges logarithmically as Ω approaches $\pm2\Delta$: $\chi''_0(\Omega)\propto\log[\Delta/\sqrt{\Omega^2-4\Delta^2}]$.

The corresponding real part at small frequencies varies as $\chi'_0(\Omega)=N_0[1+O(\Omega^2/\Delta^2)]$, with N_0 the density of states at the Fermi level, and increases up to 2Δ before discontinuously jumping across zero at a frequency of twice the maximal gap on the Fermi surface. A milder jump occurs at twice the energy at $\mathbf{k}=(\pi/a,0)$ and equivalent van Hove points. We plot $\chi'_0(\Omega)$ in Fig. 1, using $\Delta_0=35$ meV and the band struc-

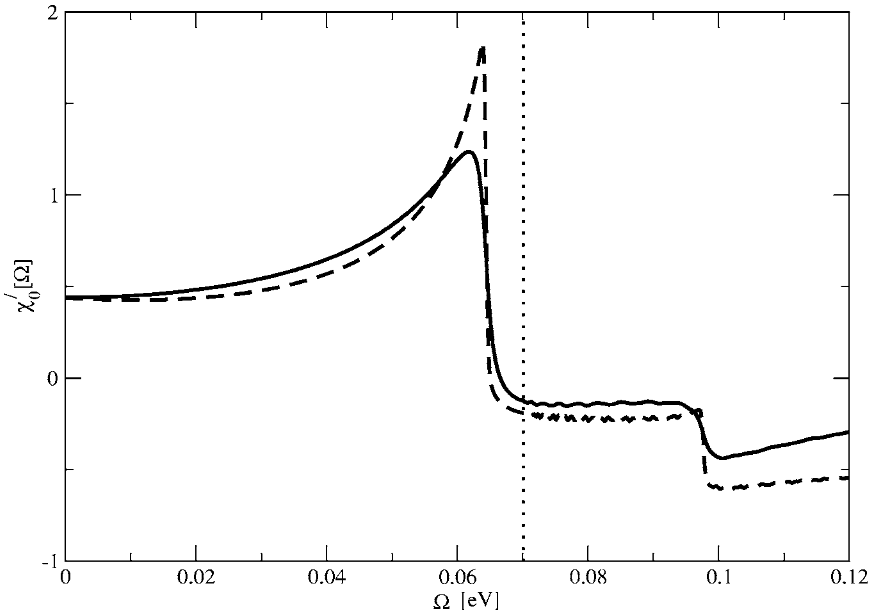

FIG. 1. The real part of the B_{1g} Raman response in the superconducting state χ_0' for the case of small fermionic damping (solid line) and no fermionic damping (dashed line). The vertical dotted line marks $2\Delta_0$. A small change between $2\Delta_0$ and the frequency where $\chi_0'(\Omega)$ is peaked is due to the fact that the maximum value of the gap $\Delta(\mathbf{k})$ along the Fermi surface is slightly smaller than Δ_0.

ture ϵ_k given by Ref. 9 to fit angle-resolved photoemission data on optimally doped $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212). Although the generic behavior changes near $2\Delta_0$ if damping (phenomenologically represented by δ) is increased, the rapid rise and fall of the real part near 2Δ is preserved.

The interaction V_{pair} has two effects on the Raman response: self-energy renormalization of the fermions in the particle-hole bubble and renormalization of the vertex. Self-energy renormalization does not distinguish qualitatively between phonons and spin fluctuations and still preserves the peak $I_{B_{1g}}(\Omega)$ at $\Omega = 2\Delta$. Renormalization of the B_{1g} vertex is more relevant. There is no spin-induced sign change between vertex renormalization due to phonons and due to spin fluctuations: Convoluting the spin dependence of $V^{pair}_{\alpha\beta,\gamma\delta}$ with $\delta_{\beta\gamma}$ of the Raman vertex $\Gamma_{\beta\gamma}(k)$, we find that for magnetic interaction, the summation over spin indices yields $\delta_{\beta\gamma}\sigma_{\alpha\gamma}\sigma_{\beta\delta} = \Sigma_i(\sigma^2_{\alpha\delta})_i = 3\delta_{\alpha\delta}$, while for phonons, $\delta_{\beta\gamma}\delta_{\alpha\gamma}\delta_{\beta\delta} = \delta_{\alpha\delta}$. In both cases, the spin configuration and sign of the Raman vertex are reproduced. Summing up the vertex correction diagrams in the ladder approximation, we obtain

$$I^{ph}_{B_{1g}}(\Omega) = \Gamma^2 \frac{\chi_0''(\Omega)}{[1 + (1/2)V_{ph}\chi_0'(\Omega)]^2 + [(1/2)V_{ph}\chi_0''(\Omega)]^2}$$

$$I^{spin}_{B_{1g}}(\Omega) = \Gamma^2 \frac{\chi_0''(\Omega)}{[1 + (3/2)V_{spin}\chi_0'(\Omega)]^2 + [(3/2)V_{spin}\chi_0''(\Omega)]^2}. \tag{3}$$

Recall that V_{spin} must be negative, and V_{ph} must be positive, if each is to give d-wave pairing. The sign of the vertex renormalization in (3), then, *is different for phonons and spin fluctuations*. Recall that $\chi_0''(\Omega)$ in the superconducting state is quite small except for Ω near 2Δ. The renormalization of the Raman vertex at $\Omega < 2\Delta$ comes mostly from χ_0'.

Since χ_0' is positive, vertex renormalization due to phonons reduces the Raman vertex at small frequencies and only slightly shifts up the peak which remains close to 2Δ. On the other hand, if the d-wave interaction is magnetic in origin, $V_{spin}\chi_0'(\Omega) < 0$, and for strong enough V_{spin}, there exists a frequency $\Omega_{res} < 2\Delta$ at which $(3/2)V_{spin}\chi_0'(\Omega_{res}) = -1$. At this frequency, $I^{spin}_{B_{1g}}$ has a peak; i.e., the B_{1g} Raman intensity develops a resonance. Because $\chi_0''(\Omega)$ is nonzero at any $\Omega > 0$, the peak is not infinitely sharp as in an s-wave superconductor.[10] However, because $\chi_0'' \propto \Omega^3$ at small frequencies, the width of the peak is small if Ω_{res} is substantially smaller than 2Δ. This resonance was discovered in Ref. 11, although its origin was not discussed in detail.

We plot in Fig. 2 the full B_{1g} Raman response for $T=0$ in the superconducting state for different values of the interaction V_{ch} and V_{spin}, using the parameters shown for Fig. 1. With no vertex corrections ($V=0$), the Raman response rises as Ω^3 and has a clear peak at twice the gap and another smaller peak at twice the van Hove energy. For magnetic interactions $V < 0$, the low-energy peak sharpens and moves to lower frequency as the resonance develops and steals spectral weight from the 2Δ feature. Two separate peaks do not develop, but the original 2Δ peak shifts down as the interaction increases. Conversely, for phononic interactions $V > 0$, the peak renormalizes upwards and weakens. No low-energy resonance develops.

The B_{1g} Raman resonance is similar to the resonance in the spin susceptibility in a d-wave superconductor.[4] In both cases, the d-wave symmetry of the gap is crucial, and the resonance emerges due to residual attraction between fermions and spin fluctuations. The neutron resonance is virtually a bound state in the sense that it is infinitesimally narrow. Because the real part of the bare spin susceptibility $\chi_s(Q,\Omega)$, where $Q = (\pi/a, \pi/a)$, evolves between 0 and infinity at $0 < \Omega < 2\Delta$, whereas $\chi_s''(Q,\Omega) = 0$, V_{spin} is not required to exceed a threshold. This is so because the spin susceptibility at momentum Q is determined by fermions near hot spots, where k and $k+Q$ are both near the Fermi surface. The hot spots are generally located away from the nodes; hence, in the superconducting state hot fermions are fully gapped, and a spin fluctuation needs a finite energy to be able to decay

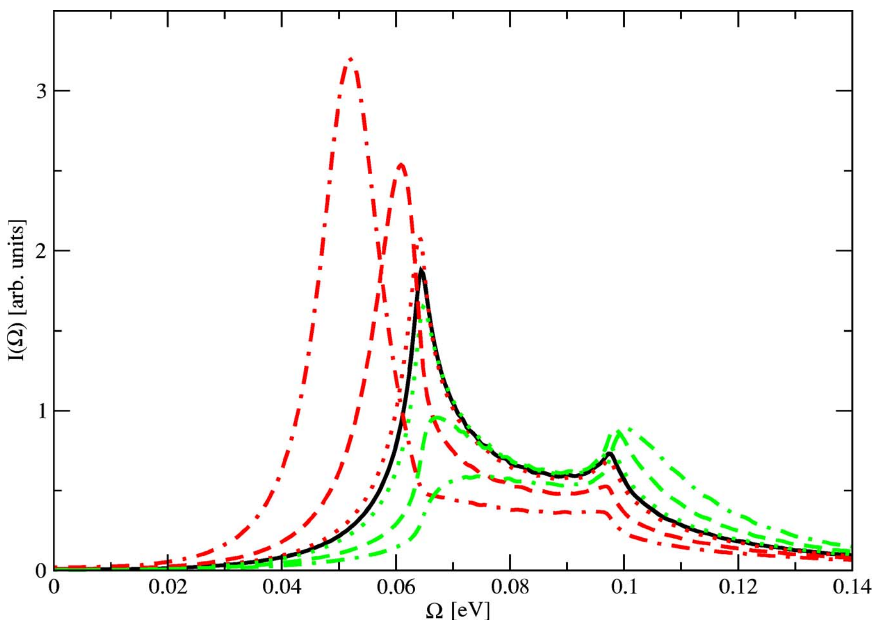

FIG. 2. (Color online) The full Raman response plotted for $VN_0=0$ (black solid line), and $\pm 0.01, 0.1, 0.5$ (dotted, dashed, dashed-dotted lines, respectively) for phonon-mediated ($V=V_{ph}$, green lines) and spin-mediated ($V=V_{spin}$, red), respectively.

into a particle-hole pair. The Raman resonance is a $Q=0$ probe and therefore involves fermions from the entire Fermi surface, including nodal regions. The fermions near the nodes account for a nonzero $\chi_0''(\Omega)$ at any finite Ω and therefore give an intrinsic width to the Raman resonance peak. The interaction then should be above the threshold for the resonance to become visible.

We now extend the analysis in three ways. First, when V_{spin} and V_{ph} are both nonzero, the resonance condition becomes $(1/2)V_{eff}\chi_0'(\Omega)=-1$, with $V_{eff}=3V_{spin}+V_{ph}$. Since $V_{spin}<0$ and $V_{ph}>0$ both favor d-pairing, they compete to determine V_{eff}. Thus the full B_{1g} Raman response (Fig. 2) is a function of the net pairing interactions V_{eff}, and the presence of the resonance requires $3V_{spin}>|V_{phonon}|$ if d-pairing occurs via both channels.

Second, the analysis can be extended to the case in which pairing interaction and the Raman vertex are not identical. The explicit form of the bare Raman vertex $\gamma_{\mathbf{k}}$ depends on many details. For instance, if the incident photon energy E_i lies near the energy of optically active electronic transitions, $\gamma_{\mathbf{k}}$ may acquire dependence on E_i as well as wave vector $\mathbf{k}$ ("resonance-Raman effect").[12] For cuprates, this might increase $|\gamma_{\mathbf{k}}|$; e.g., in B_{1g} symmetry near the antinodes. Let $V^{pair}(\mathbf{k}-\mathbf{p}) \propto \phi_{\mathbf{k}}\phi_{\mathbf{p}}$. The Raman intensity at temperature T becomes

$$I(\Omega) \sim \mathrm{Im}\, \Delta_0^2 \left[\frac{K_{11} + \eta(K_{11}K_{00} - K_{10}K_{01})}{1 + \eta K_{00}} \right]. \quad (4)$$

Here the gap $\Delta(k)=\Delta_0\phi_k$, $\eta=2\Delta_0^2(3V_{spin}+V_{ph})$,

$$K_{nm}(\Omega,T) = \int \frac{d^2k}{(2\pi)^2} \frac{(\phi_{\mathbf{k}})^{4-n-m}\gamma_{\mathbf{k}}^n(\gamma_{\mathbf{k}}^*)^m}{E_{\mathbf{k}}[4E_{\mathbf{k}}^2 - (\Omega + i\delta)^2]} \tanh \frac{E_{\mathbf{k}}}{2T}, \quad (5)$$

and $E_{\mathbf{k}}^2=\epsilon_k^2+\Delta_0^2\phi_{\mathbf{k}}^2$. When $\gamma_k=\phi_k$, $K_{nm}=K_{00}=(1/4\Delta_0^2)\chi_0(\Omega)$ and Eq. (4) coincides with Eq. (3). If ϕ_k and γ_k belong to different IR, $K_{10}K_{01}$ vanishes by symmetry, and $I(\Omega) \sim \mathrm{Im}\, \Delta_0^2 K_{11}$, i.e., there is no resonance. If ϕ_k and γ_k have the same symmetry, but are not identical, the resonance exists, but its residue depends on the strength of the $K_{10}K_{01}$ term.

Third, we argue that for spin mediated d-wave pairing, the resonance in the B_{1g} channel survives even when the effective interaction includes a dynamic term, e.g., Landau damping, and vanishes at high frequency. The real part of the vertex renormalization, which accounts for the resonance, comes partly from fermions with high frequencies. Once the interaction vanishes at high frequency, this part disappears. Will the remaining part still have the same sign?

To answer this question, we computed $V_{spin}\chi_0(\Omega)$ in Eliashberg theory, which includes Landau damping. The computational procedure is rather involved, and we just cite the result. We obtained the expression for the Raman vertex renormalization $\Gamma_{B_{1g}}(\Omega)=\Gamma d_k/[1-J(\Omega)]$ by first summing up the series of vertex corrections in Matsubara frequencies, and then analytically continuing to the real axis by introducing double spectral representation. The quantity $J(\Omega)$ replaces $|V_{spin}|\chi_0(\Omega)$ in Eq. (3). We found that now $J(0)=0$, in contrast to the case of the constant interaction, where $\chi_0(0)\neq 0$, but still $J'(\Omega)>0$ at $\Omega<2\Delta$ and it is peaked at 2Δ. Thus, vertex corrections, even without a high frequency term, still lead to a resonance in $I(\Omega)$ at some $\Omega<2\Delta$.

The only extensive set of data comparing B_{1g} symmetry Raman gap values with those from the single electron spectroscopies of angle-resolved photoemission spectroscopy (ARPES) and tunneling is found for the $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212) family. Values found by five groups for the Raman gap in terms of the hole doping p are shown in Fig. 3. The Raman gap values are compared in this figure with those from tunneling and ARPES. Tunneling results are from Ref. 13 and represent peak-to-peak separations in positive and negative biases. ARPES results are from Ref. 14. For completeness, we presented twice the gap Δ determined from two sets of ARPES data: the position of the peak at $(0,\pi)$, and the midpoint of the leading edge gap inferred from several different forms of modeling.

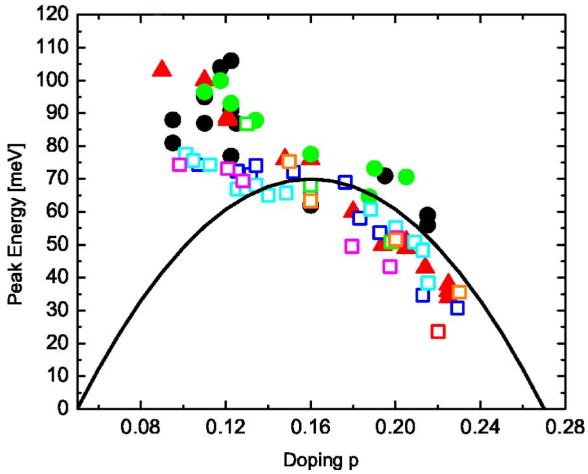

FIG. 3. (Color online) The Raman data (open squares) from five different groups [Ref. 23 (red), Ref. 15 (magenta), Ref. 20 (orange), Ref. 21 (green), Ref. 16 (blue), Ref. 17 (cyan), respectively], together with the tunneling data (red triangles) from Ref. 13 and ARPES data from Ref. 14. (Black circles are derived from leading edge spectra while green circles are from the peak position of the $\pi,0$ spectra.) The doping p was determined by the formula $p=0.16\pm\sqrt{\frac{|T_c-T_c^{max}|}{82.6T_c^{max}}}$, where T_c is the superconducting transition temperature. The solid line plots 70 meV (T_c/T_c^{max}).

For doping p greater than 0.2, well-defined peaks emerge below T_c in the B_{1g} channel at a frequency roughly consistent with the tunneling gap. Both Raman and tunneling data fall below rather scattered ARPES data. The agreement between Raman and tunneling results indicates that the B_{1g} vertex renormalization is small in the overdoped regime. This may be the consequence of just small enough spin-fermion coupling, or the partial cancellation between the renormalizations due to spin fluctuations and to phonons. The distinction with ARPES is likely due to ARPES resolution and also, possibly, to the effects from bilayer splitting.[24,25]

For p less than or equal to the optimal value of 0.16, the Raman gap values in Fig. 3 are mostly from Refs. 15–17. They fall consistently below those from tunneling and from ARPES, although there is some degree of scatter. For the Raman work, the used photon energies were 2.0 or 2.4 eV. Small (8%–10%) resonance-Raman effects on the B_{1g} peak position seen at higher dopings within the 2–3 eV range[18,19] would not change this conclusion. In regard to the findings of this paper, this implies that the pairing more likely arises from spin fluctuations in the underdoped range. Yet the growth of intensity predicted in Fig. 2 is not seen. This may be a result of inelastic scattering or may be due to the presence of the pseudogap (PG). For a Raman calculation using one model for the PG. In addition, for reasons that are not well understood, other groups[20,21] find very weak B_{1g} Raman signals from underdoped samples of Bi2212. They thus find it difficult to impossible to extract values of 2Δ in this symmetry and doping range.

Yet this is not the case for B_{2g} scattering (light orientations rotated by 45° with respect to B_{1g} orientations). Peaks have been shown to occur only at temperatures below T_c at a frequency that scales with T_c *for all dopings*.[22] This apparent contradiction between the findings in B_{1g} and B_{2g} must be reconciled before firm conclusions can be drawn about the pairing mechanism. A possible alternative scenario could be that the antinodal quasiparticles become gapped via a mechanism not related to superconductivity, such as precursor spin- or charge-density wave formation. In this case, the difference in values of 2Δ from B_{1g} Raman, ARPES, and scanning tunneling microscopy and other probes would not be unexpected. This open question merits further investigation.

To conclude, we considered B_{1g} Raman intensity in a d-wave superconductor. With interactions neglected, this is peaked at 2Δ, but for interacting fermions there is a qualitative distinction between spin-mediated and phonon-mediated cases. For spin-mediated interaction, the peak in the intensity shifts downwards due to the development of the resonance below 2Δ. The resonance survives even if the interaction is retarded. For phonon (or other charge-mediated) interaction, the resonance does not develop, and a weakened peak remains at 2Δ. We also considered the case in which the pairing interaction and the Raman vertex have the same symmetry, but are not identical, and showed that photon resonance-Raman effects might change the residue of the B_{1g} resonance.

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