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.

This paper is devoted to the analysis of whether there exists an observable that would distinguish between magnetically mediated and phonon-mediated $d$–wave superconductivity. This subject is motivated by the cuprates for which recent measurements, particularly the observation of the kink in the quasiparticle dispersion [1], has revived the discussion of whether the pairing in the quasiparticle dispersion. Thus, to truly distinguish between the two scenarios, one needs to identify an observable for which phonon and spin-fluctuation pairings yield qualitatively different results.

In this communication, we argue 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 $\omega_{res} < 2\Delta_{max}$, while in phonon-mediated $d$–wave superconductors, such a resonance does not develop. The resonance is excitonic in origin, and is similar to the excitonic resonance in the spin susceptibility of a $d$–wave superconductor [4]. The only difference is that the resonance in $B_{1g}$ Raman scattering comes from fermions all around the Fermi surface and has a finite intrinsic width because of the nodes, whereas the resonance term in the spin susceptibility comes only from fermions in the antinodal regions and is a true, $\delta$–functional bound state.

To make the argumentation straightforward, we first consider the simplest case of $S = 1/2$ fermions interacting via a static potential $V_{pair}(k)$

$$\mathcal{H}_{int} = -\sum_{q,k,p} \psi_{k,a}^\dagger(1) \psi_{p+q,a}^\dagger V_{pair}^{\alpha\beta,\gamma\delta}(k-p) \psi_p \psi_q$$

In Eq. (1) summation over spin indices $\alpha, \beta, \gamma$ and $\delta$ is understood. As $B_{1g}$ vertex has the same $d$–wave form as the pairing gap, we further approximate $V_{pair}$ by its $d$–wave component $V_{pair}(k-p) \propto d_k d_p$, where $d_k = [\cos(k_x a) - \cos(k_y a)]/2$.

The effective interaction $V_{\alpha\beta,\gamma\delta}^{\text{pair}}(k-p)$ may be due to spin fluctuations or to phonons. For spin mediated interaction, $V_{\alpha\beta,\gamma\delta}^{\text{pair}}(k-p) = V_{\text{spin}} d_k d_p \sigma_{\alpha\beta} \cdot \sigma_{\gamma\delta}$ where $\sigma$ are Pauli matrices. For phonon-mediated interaction $V_{\alpha\beta,\gamma\delta}^{\text{pair}}(k-p) = V_{\text{ph}} \sigma_{\alpha\beta} \delta_{\gamma\delta}$. We assume that both interactions lead to a $d$–wave pairing, and study the consequences for the Raman intensity. From this perspective, our results are equally applicable if phonons are replaced by charge density waves [2].

Our first observation is that the signs of $V_{\text{spin}}$ and $V_{\text{charge}}$ must be different, if they both lead to an attraction in a $d$–wave channel. Indeed, substituting effective interactions into the diagrammatic expression for the $d$–wave, spin-singlet pairing vertex $\psi^\dagger_{k,\alpha} \Phi_d(k) \psi^\dagger_{-k,\beta}$, where $\Phi_d(k) = \Phi_d^0 k \alpha^\dagger$, and using $\sigma^\dagger_{\alpha\gamma} \delta_{\alpha\gamma} \delta_{\delta\beta} = \sigma^\dagger_{\beta\delta}$, $\sigma_{\alpha\beta} \sigma_{\gamma\delta} = -3d^\dagger_{\gamma\delta}$, we obtain that $\Phi$ is related to the bare vertex $\Phi_0$ as

$$\Phi = \frac{\Phi_0}{1 + 3AV_{\text{spin}}}; \Phi = \frac{\Phi_0}{1 - AV_{\text{ph}}}$$

for spin-mediate or phonon-mediated interaction, respectively. A positive $A \propto \log(\omega_{c})$ is a conventional logarithmic cut-off factor. To get an attraction, one then obviously needs $V_{\text{ph}}$ to be positive, $V_{\text{spin}}$ to be negative. This is the case when phonon mediated interaction is peaked at small momenta, and spin-mediated interaction is peaked at momenta near $(\pi, \pi)$ [2].

Suppose next that the system is a $d$–wave superconductor, either due to phonons or due to spin fluctuations. Consider how this affects the Raman response in the $B_{1g}$ channel. The $B_{1g}$ Raman vertex $\Gamma_{\alpha\beta}(k)$ has $d$–wave momentum dependence and is a spin scalar: $\Gamma_{\alpha\beta}(k) = \Gamma_d^0 k_{\alpha\beta}$. For a BCS superconductor without vertex or self energy corrections, the $B_{1g}$ Raman intensity $I_{B_{1g}}(\Omega) = \Gamma^2 I m \chi_0(\Omega)$ and $\chi_0(\omega)$ is the imaginary part of the particle-hole bubble with two $d$–wave vertices (see e.g. Ref. [3]). In the normal state, $\chi_0(\Omega)$ vanishes, as it should as there is no low-energy phase-space available for scattering with $q = 0$. In the superconducting state, light can break Cooper pairs with $q = 0$ and $\chi_0(\Omega)$ is given by Tsumura function weighted with $d_k^2$ [3]. The imaginary part of $\chi_0(\Omega)$ scales as $\Omega^2$ at small frequencies [4], and diverges logarithmically as $\Omega$ approaches $\pm 2\Delta$: $\Im \chi_0(\Omega) \propto \log\Delta/\sqrt{\Omega^2 - 4\Delta^2}$.
The corresponding real part at small frequencies varies as \( \text{Re} \chi_0(\Omega) = N_0[1 + O(\Omega^2/\Delta^2)] \), with \( N_0 \) the density of states at the Fermi level, and keeps increasing up to \( 2\Delta \) before discontinuously jumping across zero at a frequency of twice the maximal gap on the Fermi surface. Another milder jump occurs at twice the energy at the van Hove points at \( (\pi, 0) \) and related points in the Brillouin zone. We plot \( \text{Re} \chi_0(\Omega) \) in Fig. 1 using \( \Delta_0 = 35 \) meV and the band structure \( \epsilon_k \) given by Eschrig and Norman\(^{10} \) to fit the angle-resolved photoemission (ARPES) on optimally doped \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x} \) (Bi-2212). Although the generic behavior changes near \( 2\Delta_0 \) if damping (phenomenologically represented by \( \delta \)) is increased, the rapid rise and fall of the real part near \( 2\Delta \) is preserved.

Consider now what happens to the Raman response when we add \( V_{\text{pair}} \). This interaction leads to two effects - self-energy renormalization of the fermions in the particle-hole bubble, and the renormalization of the Raman vertex. The self-energy renormalization does not distinguish qualitatively between phonons and spin fluctuations, and still preserves the peak \( I_{B_{1g}}(\Omega) \) at \( \Omega = 2\Delta \). The renormalization of the \( B_{1g} \) vertex is more relevant.

To understand its role we first observe that there is no spin-induced sign change between vertex renormalization due to phonons and due to spin fluctuations. Indeed, convoluting the spin dependence of \( V_{\text{pair}} \) with \( \delta_{\beta\gamma} \) of the Raman vertex \( \Gamma_{\beta\gamma}(k) \), we find that for magnetic interaction, the summation over spin indices yields \( \delta_{\beta\gamma} \sigma_{\alpha\gamma} \sigma_{\beta\delta} = \sum_i (\sigma_{\alpha\delta})_i = \delta_{\alpha\delta} \), while for phonons \( \delta_{\beta\gamma} \omega_{\alpha\gamma} \delta_{\beta\delta} = \delta_{\alpha\delta} \). As a result, in both cases, the spin configuration of the Raman vertex is reproduced, and the sign is the same in both cases. Summing up the vertex correction diagrams in the ladder approximation, we obtain

\[
I_{B_{1g}}^{\text{ph}}(\Omega) = \Gamma^2 \frac{\chi''_0(\Omega)}{(1 + \frac{1}{2} V_{\text{ph}} \chi'_0(\Omega))^2 + \left(\frac{1}{2} V_{\text{ph}} \chi''_0(\Omega)\right)^2}
\]

\[
I_{B_{1g}}^{\text{spin}}(\Omega) = \Gamma^2 \frac{\chi''_0(\Omega)}{(1 + \frac{1}{2} V_{\text{spin}} \chi'_0(\Omega))^2 + \left(\frac{1}{2} V_{\text{spin}} \chi''_0(\Omega)\right)^2}
\]

We defined \( \chi' = \text{Re} \chi, \chi'' = \text{Im} \chi \). We now recall that \( V_{\text{spin}} \) must be negative, and \( V_{\text{ph}} \) must be positive, if each of them gives rise to a \( d^- \)-wave pairing. Then, the sign of the vertex renormalization in \( \chi'' \) is different for phonons and spin fluctuations. As mentioned above, \( \text{Im} \chi_0(\Omega) \) in the superconducting state is quite small except for near \( 2\Delta \). The renormalization of the Raman vertex at \( \Omega < 2\Delta \) then predominantly comes from \( \text{Re} \chi_0 \).

Since \( \text{Re} \chi_0(\Omega) \) 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 \( 2\Delta \). On the other hand, if the \( d^- \)-wave interaction is magnetic in origin, \( V_{\text{spin}} \chi_0(\Omega) < 0 \), and for strong enough \( V_{\text{spin}} \), there exists a frequency \( \Omega_{\text{res}} < 2\Delta \) at which \( (3/2)V_{\text{spin}} \chi_0(\Omega) = -1 \). At this frequency, \( I_{B_{1g}}^{\text{spin}} \) has a peak. Because \( \chi''_0(\Omega) \) is nonzero at any \( \Omega > 0 \), the peak is not infinitely sharp as in an \( s^- \)-wave superconductor\(^{11} \). However, since \( \chi''_0(\Omega) \propto \Omega^3 \) at small frequencies, the width of the peak is small if \( \Omega_{\text{res}} \) is substantially smaller than \( 2\Delta \). We see therefore that for spin-mediated \( d^- \)-wave pairing, the \( B_{1g} \) Raman intensity develops a resonance. The resonance for spin-mediated pairing was discovered in Ref. \(^{12} \), although its origin was not discussed in detail there. We plot in Figure 2 the full \( B_{1g} \) Raman response for \( T = 0 \) in the superconducting state for different values of the interaction \( N_0 V \) using the parameters shown for Figure 1. In the absence of interactions \( (V = 0) \) the Raman response rises as \( \Omega^3 \) 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 \( 2\Delta_0 \) feature. In agreement with Ref. \(^{12} \), two separate peaks do not develop, but because of resonance, the original \( 2\Delta \) peak progressively shifts down from \( 2\Delta \) as the interaction increases. Conversely, for phononic interactions \( V > 0 \), the peak renormalizes upwards from the final-state interactions and weakens for stronger interactions. No low energy resonance develops.

The resonance in the \( B_{1g} \) Raman response is in many respects 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 in a \( d^- \)-wave superconductor. The only difference between the two resonances is that the neutron resonance is virtually a bound state in the sense that it is infinitesimally narrow, and does not require coupling to be above a threshold because the real part of

FIG. 1: The real part of the \( B_{1g} \) Raman response in the superconducting state \( \text{Re} \chi_0 \) 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 \( \text{Re} \chi_0(\Omega) \) is peaked is due to the fact that the maximum value of the gap along the Fermi surface is slightly smaller than \( \Delta_0 \).
A Raman intensity near the resonance at a temperature \( T \) is given by
\[
\frac{\phi_k}{V} \text{ the resonance requires } 3 V \text{ directions. First, when the threshold for the resonance to become visible. }
\]

The bare spin susceptibility \( \chi_s(Q, \Omega) \), where \( Q = (\pi, \pi) \), evolves between 0 and infinity at \( 0 < \Omega < 2\Delta \), where \( \text{Im} \chi_s(Q, \Omega) = 0 \). This comes about 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 gaped, and a spin fluctuation needs a finite energy to be able to decay into a particle-hole pair. The Raman resonance, on the other hand, is a \( Q = 0 \) probe. It therefore involves fermions from the entire Fermi surface, including nodal regions. The nodal fermions account for a nonzero \( \text{Im} \chi_0(Q, \Omega) \) at any finite \( \Omega \) and therefore produce an intrinsic width of the Raman resonance peak. The interaction then should be above the threshold for the resonance to become visible.

We now extend the above analysis in several different directions. First, when \( V_{\text{spin}} \) and \( V_{\text{ph}} \) are both nonzero, the resonance condition becomes \( (1/2)V_{\text{eff}} \chi_0(Q, \Omega) = -1 \), with \( V_{\text{eff}} = 3V_{\text{spin}} + V_{\text{ph}} \). We remind the reader that \( V_{\text{spin}} < 0 \) and \( V_{\text{ph}} > 0 \) both favor \( d \)-pairing, and thus they compete to determine \( V_{\text{eff}} \). Thus referring back to Figure 2 the full \( B_{1g} \) Raman response is a function of the net pairing interactions \( V_{\text{eff}} \), and the presence of the resonance requires \( 3V_{\text{spin}} > |V_{\text{photon}}| \) if \( d \)-pairing occurs via both channels.

Second, the analysis can be extended to the case where the pairing interaction and the Raman vertex have the same symmetry, but are not identical. If \( V_{\text{pair}}(k-p) \propto \phi_k \phi_p \) and the bare Raman vertex is \( \Gamma_k = \Gamma_{\gamma k} \), where the functions \( \phi_k \) and \( \gamma_k \) belong to the same irreducible representation different from fully symmetric \( A_{1g} \), the RPA Raman intensity near the resonance at a temperature \( T \) is given by

\[
I_{\gamma k}(\Omega) \sim \text{Im} \left[ \frac{\Delta^2 K_{10}K_{01}}{1 + 2\Delta^2 (3V_{\text{spin}} + V_{\text{ph}})K_{00}} \right]
\]

for spin and phonon mediated pairing, where

\[
K_{n,m}(\Omega, T) = \int \frac{d^2 k}{(2\pi)^2} \frac{(\phi_k)^{4-n}m_{\gamma}m_{\phi}^{m}}{E_k(4E_k^2 - (\Omega + i\delta)^2) + \alpha_k E_k^2} \tanh \frac{E_k}{2T} \tag{5}
\]

and \( E_k^2 = \epsilon_k^2 + \Delta^2 \phi_k^2 \). One can verify that for \( \phi_k = d_k, K_{00}(\Omega, 0) = K_{10}(\Omega, 0) = K_{01}(\Omega, 0) = (1/4\Delta^2)\chi_0(\Omega) \), and \( K \) coincides with \( \chi_0(\Omega) \). Eq. 5 however shows that once \( 3V_{\text{spin}} + V_{\text{ph}} \) is negative, the resonance occurs for any pairing symmetry different from \( A_{1g} \), for the Raman vertex for which \( K_{01} \) and \( K_{10} \) are finite.

Third, we argue that for spin mediated pairing \( d \)-wave pairing, the resonance in the \( B_{1g} \) channel survives even when the effective interaction includes a dynamic term, e.g., the Landau damping, and vanishes at high frequencies. The vanishing of \( V_{\text{pair}}(k, \omega) \) at large \( \omega \) may have a profound effect on the renormalization of the vertex at zero momentum transfer as the real part of the vertex renormalization, which accounts for the resonance in our case, partly comes from fermions with high frequencies. Once the interaction vanishes at high frequencies, this part disappears, and it becomes an issue whether the remaining part still has the same sign.

To address this issue, we computed \( V_{\text{spin}} \chi_0(\Omega) \) in Eliashberg theory which includes Landau damping. We obtained the expression for the Raman vertex renormalization \( \Gamma_{\text{B}_{1g}}(\Omega) = \Gamma_{dk}(1 + J(\Omega)) \) by first evaluating the vertex correction in Matsubara frequencies, and then analytically continuing to the real axis by introducing double spectral representation. We found that \( J(0) = 0 \), but \( J(\Omega) < 0 \) at \( \Omega \approx 2\Delta \) still logarithmically diverges at \( 2\Delta \), i.e., vertex corrections, even without high frequency term, still increase the Raman vertex and lead to a resonance in \( R(\Omega) \) 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 \( Bi_2Sr_2CaCu_2O_{8+\delta} \) (“Bi-2212”) family. Values found by five groups for the Raman gap in terms of the hole doping \( p \) are shown in Figure 3. The Raman gap values are compared in this figure with those from tunneling and ARPES. Tunneling results are from Ref [24] and represent peak-to-peak separations in positive and negative biases. ARPES results are from Ref [22]. For completeness, we presented twice the gap \( \Delta \) determined from two sets of ARPES data - the position of the peak at \((0, \pi)\), and the mid-point of the leading edge gap inferring from several different forms of modelling.

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 con-
from $B_{1g}$ Raman, ARPES, and STM and other probes would not be unexpected. This remains very much an open question meriting further investigation.

To conclude, in this paper, we considered $B_{1g}$ Raman intensity in a $d$–wave superconductor. For non-interacting fermions, $B_{1g}$ intensity is peaked at $2\Delta$. We found that for interacting fermions, there is a qualitative distinction between spin-mediated and phonon-mediated interactions. For spin-mediated interaction, the peak in the intensity shifts downwards compared to $2\Delta$ due to the development of the resonance below $2\Delta$. We verified that the resonance survives even if the interaction is retarded. For phonon-mediated interaction, the resonance does not develop, and the peak remains at $2\Delta$. The effect is quite generic and is also valid if phonons are replaced by charge-density-waves. We presented the generic condition under which resonance occurs in a Raman vertex of arbitrary symmetry.

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References

[1] P. V. Bogdanov et al., Phys. Rev. Lett. 85, 2581 (2000); A. Lanzara et al., Nature (London) 412, 510 (2001); A. Kaminski et al., Phys. Rev. Lett. 86, 1070 (2001); P. D. Johnson et al., Phys. Rev. Lett. 87, 177007 (2001); X. J. Zhou et al., Nature (London) 423, 398 (2003); A. D. Gromko et al., Phys. Rev. B 68, 174520 (2003); T. Sato et al., Phys. Rev. Lett. 91, 157003 (2003); T. Cuk et al., Phys. Rev. Lett. 93, 117003 (2004); A. Kordyuk, Phys. Rev. B 71, 214513 (2005).

[2] T. P. Devereaux et al., Phys. Rev. Lett. 93, 117004 (2004); T. Cuk et al., Phys. Stat. Sol. (b) 242, 11 (2005).

[3] A. V. Chubukov and M. R. Norman, Phys. Rev. B 70, 174505 (2004).

[4] see e.g., M. R. Norman, Phys. Rev. B 61, 14751 (2000) and references therein

[5] G. Seibold and M. Grilli, cond-mat/0409506

[6] See e.g., P. Monthoux, A. Balatsky and D. Pines, Phys. Rev. B 46, 14803 (1992) and N. Bulut and D. J. Scalapino, Phys. Rev. B 54, 14971 (1996), Ar. Abanov, A. V. Chubukov, J. Schmalian, Journal of Electron Spectroscopy and Related Phenomena 117, 129 (2001).

[7] T. P. Devereaux

[8] M. V. Klein and S. B. Dierker, Phys. Rev. B 29, 4976 (1984).

[9] T. P. Devereaux, D. Einzel, B. Stadlober, R. Hackl, D. H. Leach, and J. J. Neumeier, Phys. Rev. Lett. 72, 396 (1994).

[10] M. Eschrig and M. R. Norman, Phys. Rev. Lett. 85, 3261 (2000).

[11] H. Monien and A. Zawadowski, Phys. Rev. B 41, 8798 (1990).

[12] A. Chubukov, D. Morr, and G. Blumberg, Solid State Comm. 112, 193 (1999).
[13] T. Masui, M. Limonov, H. Uchiyama, S. Lee, S. Tajima, and A. Yamanaka, Phys. Rev. B 68, 060506 (2003) and references therein.

[14] A. Damascelli, Z. Hasid, and Z.-X. Shen, Rev. Mod. Phys. 75, 473 (2004); Ch. Renner et al., Phys. Rev. Lett. 80, 149 (1998); D.L. Feng et al., Phys. Rev. Lett. 86, 5550 (2001).

[15] G. Blumberg et al., Science 278, 1427 (1997); J. Phys. Chem. Solids 59, 1932 (1998).

[16] F. Venturini et al., Phys. Rev. Lett. 89, 107003 (2002).

[17] M. Opel et al., Phys. Rev. B 61, 9752 (2000).

[18] K. C. Hewitt and J. C. Irwin, Phys. Rev. B 66, 054516 (2002), especially Figs. 1 and 2 and Table II.

[19] C. Kendziora and A. Rosenberg, Phys. Rev. B 52, 9867 (1995).

[20] G. Blumberg et al., Science 278, 1427 (1997); G. Blumberg et al., J. Phys. Chem. Solids 59, 1932 (1998). The $T_c = 65K$ result was not used because it has only the narrow 75 meV peak.

[21] T. Staufer et al., Phys. Rev. Lett. 68, 1069 (1992); M. Opel et al., Physica B 284-288 (2000); R. Hackl et al., Proc. SPIE 2696, 194 (1996); F. Venturini et al., J. Phys. Chem. Solids 63, 2345 (2002).

[22] S. Sugai and T. Hosokawa, Phys. Rev. Lett. 85, 1112 (2000), Fig. 2. The $T_c = 75K$ result was not used because the gap feature, if present, was extremely weak.

[23] J. C. Compuzano et al., Phys. Rev. Lett. 83, 3709 (1999); H. Ding et al., Phys. Rev. Lett. 87, 227001 (2001).

[24] N. Miyakawa et al., Phys. Rev. Lett. 80, 157 (1998); Y. De Wilde et al., Phys. Rev. Lett. 80, 153 (1998); J. F. Zasadzinski, et al., Phys. Rev. Lett. 87, 067005 (2001). Most results used the SIS point-contact technique.