Dichotomy and pseudogap signature in the Raman response of high-T_c cuprates

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(Received 27 July 2009; revised manuscript received 26 January 2010; published 4 May 2010)

The signature of the pseudogap in the normal-state Raman response of high-T_c cuprates is examined within the rotating antiferromagnetism theory. The results for the B_{1g} and B_{2g} response functions, including spectral weight transfer and quasiparticle's dichotomy, compare well with experiment. A pseudogap-induced peak in the B_{1g} response is found to behave like the superconducting peak; the low-frequency B_{1g} response behaves as ω^a with $a\sim 3$ in the clean limit, and $a=1$ in the dirty limit. Also, we find that the zero-frequency slopes for both B_{1g} and B_{2g} scale as the inverse (inverse squared) of the zero-frequency scattering rate in the clean limit (dirty limit).

DOI: 10.1103/PhysRevB.81.174502 PACS number(s): 74.72.−h, 74.25.Gz, 75.10.−b

I. INTRODUCTION

Electronic Raman scattering (ERS) experiments have been used[1–15] to probe the energy scale, symmetry and temperature dependence of the pseudogap (PG) in high-T_c cuprates. In ERS experiments, one may investigate various parts of the Fermi surface by a simple choice of the incident and scattered light polarization vectors. The B_{1g} spectra sample[1,3–5] regions of the Fermi surface located near the Brillouin zone (BZ) principal axes [i.e., $(\pm\pi,0)$, $(0,\pm\pi)$], while B_{2g} spectra sample regions located near the diagonal directions [i.e., $(\pm\pi,\pm\pi)$]. Thus the B_{1g} and B_{2g} scattering geometries probe the behavior of antinodal and nodal quasiparticles (QPs), respectively.[6,7,13,16,17] In addition, the zero-frequency slopes of the B_{1g} and B_{2g} response functions, which have been found[10] to be inversely proportional to the QP scattering rate, exhibit a remarkable dichotomy. Over a wide doping range $(0.1<p<0.23)$, QPs in the B_{2g} channel display[6,15,18] metal-like transport; the scattering rate decreases with decreasing temperature. While the same is true of antinodal QPs in the heavily overdoped (OD) regime $(p>0.2)$, there are significant changes with underdoping. Over the range $0.16<p<0.2$ the (zero-frequency) antinodal QP scattering rate is temperature independent. Finally, for hole concentrations less than optimal $(p<0.16)$ the scattering rate increases with decreasing temperature, a hallmark of semiconducting/insulating behavior. This has been interpreted[15,19] in terms of an unconventional metal-insulator transition near a quantum critical point $(p\approx 0.2)$.

To explain these features one approach proposes[20,21] antiferromagnetic (AF) spin fluctuations as the basis of the dichotomy because the magnitude and direction of the AF ordering vector $\mathbf{q}=(\pi,\pi)$ allow particles lying near the BZ principle axes to exchange $\mathbf{q}$ while those along the diagonals cannot. The persistence of a two-magnon peak in the B_{1g} spectra over a wide doping range[22] provides evidence of these fluctuations. Another theory in which the PG originates in spin fluctuations is the rotating antiferromagnetism theory (RAFT).[23,24] RAFT is based on the t-t'-U Hubbard model in the normal state and has yielded promising results for resistivity,[25] Hall effect,[26] and thermodynamic properties[27] for the high-T_c cuprates. In particular, treating the QP self-energy within the marginal Fermi liquid (MFL) ansatz,[28] RAFT has successfully modeled the resistivity of La214.[25] In this work we test the applicability of RAFT by analyzing the temperature and doping dependence of the normal-state ERS response. We predict changes in the B_{1g} and the B_{2g} scattering rates as a function of disorder and find a PG-induced peak in the B_{1g} response above an isosbestic point. A recent work[29] using the Yang-Rice-Zhang model studied the ERS response in the underdoped (UD) superconducting state.

II. METHOD

The Raman scattering intensity is proportional to the imaginary part of the density-density correlation function $\chi(\mathbf{q},i\omega_m)=\int_0^\beta d\tau e^{i\omega_m\tau}\langle T_\tau\tilde{\rho}_{\mathbf{q}}(\tau)\tilde{\rho}_{-\mathbf{q}}(0)\rangle$, where $i\omega_m=i2m\pi T$ is the bosonic Matsubara frequency, τ the imaginary time, and T is temperature.[30] Following the same procedure as in Ref. 25 for the calculation of conductivity, we find the B_{1g} and the B_{2g} response functions to be

$$\chi''_{B1g}(\omega)=\int\frac{d\mathbf{k}}{(2\pi)^2}\gamma^2_{B1g}\int_{-\infty}^{+\infty}\frac{d\epsilon}{\pi}[n_F(\epsilon)-n_F(\epsilon+\omega)]\times\sum_{\nu=\pm}\left[\frac{\epsilon^2(\mathbf{k})}{E_q^2}\mathcal{L}^\nu(\epsilon)\mathcal{L}^\nu(\epsilon+\omega)+\frac{q^2}{E_q^2}\mathcal{L}^\nu(\epsilon)\mathcal{L}^{-\nu}(\epsilon+\omega)\right],\quad(1)$$

$$\chi''_{B2g}(\omega)=\int\frac{d\mathbf{k}}{(2\pi)^2}\gamma^2_{B2g}\int_{-\infty}^{+\infty}\frac{d\epsilon}{\pi}[n_F(\epsilon)-n_F(\epsilon+\omega)]\times\sum_{\nu=\pm}\mathcal{L}^\nu(\epsilon)\mathcal{L}^\nu(\epsilon+\omega),\quad(2)$$

where n_F is the Fermi-Dirac factor, $\gamma_{B1g}=t(\cos k_y-\cos k_x)$, $\gamma_{B2g}=-4t'\sin k_x\sin k_y$, $\epsilon(\mathbf{k})=-2t(\cos k_x+\cos k_y)$, and $\mathcal{L}^\pm(\xi)=\frac{\Gamma(\xi)}{[\xi+\mu'(\mathbf{k})-\Sigma'(\xi)\pm E_q]^2+\Gamma^2(\xi)}$. In the Lorentzians $\mathcal{L}^\pm$, $\Sigma'(\xi)=\mathrm{Re}\,\Sigma_r(\mathbf{k},\xi)$ and $\Gamma(\xi)=-\mathrm{Im}\,\Sigma_r(\mathbf{k},\xi)$ are the real and imaginary parts of the retarded self-energy. Here, $\mu'(\mathbf{k})=\mu$

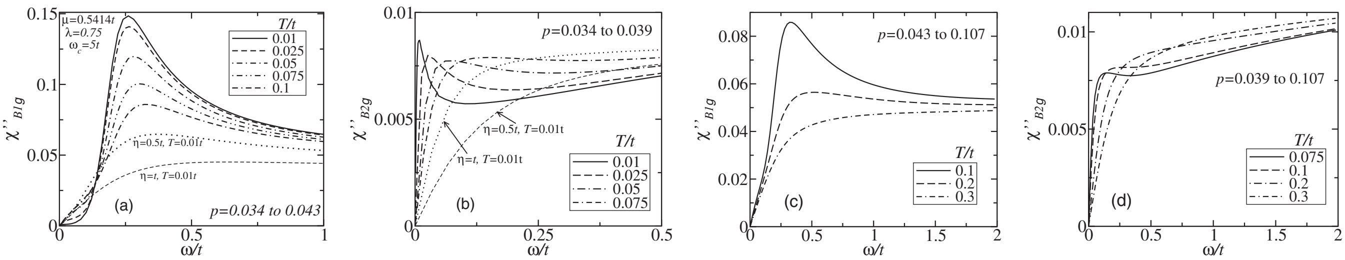

FIG. 1. The frequency dependence of χ''_{B1g} for (a) $0.01 \leq T/t \leq 0.1$ and (c) $0.1 \leq T/t \leq 0.3$; and of χ''_{B2g} for (b) $0.01 \leq T/t \leq 0.075$ and (d) $0.075 \leq T/t \leq 0.3$ is displayed for UD cuprates ($p \approx 0.03-0.1$). We used $\omega_c = 5t$ and $\lambda = 0.75$. In RAFT doping changes with T; (Ref. 26) in the UD regime, $p=0.043$ for $T=0.1t$, $p=0.071$ for $T=0.2t$, and $p=0.107$ for $T=0.3t$. In the OD regime the T effect is minor.

$+4t' \cos k_x \cos k_y - Un$ with μ the chemical potential and n the electron occupation per site and spin, and $E_q(\mathbf{k}) = \sqrt{\epsilon^2(\mathbf{k}) + q^2}$ is a gaplike energy, where $q = UQ$; Q is the rotating AF order parameter.[24,27] The normal-state QP energies in RAFT are given by $E_{\pm} = -\mu'(\mathbf{k}) \pm E_q(\mathbf{k})$.

At this point, one needs to determine self-energy Σ. Given how well the semiempirical MFL model of Varma *et al.*[28] for Σ fits existing data, like the Raman electronic background[31] and several other properties at optimal doping, we use it here. Its form is considered as an input: $\Sigma(\omega) = 2\lambda\omega \log\frac{x}{\omega_c} - i\pi\lambda x - i\eta$, where λ models the coupling of the charge carriers to the collective modes that give rise to the MFL self-energy. ω_c is a high-energy cutoff of the spectrum ($\omega_c = 5t$ here), $x = \max(|\omega|, T)$ and η is a static scattering rate. Note that deviations from the x-linear behavior in $\Sigma(\omega)$ appear in the UD regime,[32] but we ignore them; we aim to recover at least the general trends in the temperature and doping dependence of the Raman response functions, like the transfer of spectral weight and the QP dichotomy. This self-energy, with a constant λ, yields excellent fits to the experimental resistivity data for temperature greater than the PG temperature ($T > T^*$), but below T^*, λ has to be T dependent due to the PG.[25] The Hamiltonian parameters $U = 3t$ and $t' = -0.25t$ were used to obtain all the results in this paper except those in Fig. 5 where $U = 2.8t$ and $t' = -0.16t$. Our conclusions are, however, parameters independent.

III. RESULTS

Figures 1(a)–1(d) show χ''_{B1g} and χ''_{B2g} as a function of frequency ω for different temperatures in the UD regime with $\lambda = 0.75$ and zero static scattering rate; $\eta = 0$. In Fig. 1(a) a peak appears in the lowest T curves above an isosbestic point near $\omega \approx 0.30t = 30$ meV $= 240$ cm^{-1} ($t = 0.1$ eV is the value used in RAFT to fit cuprates' energy spectra). The characteristics of this PG-induced peak are similar to the pair-breaking peak observed in the B_{1g} ERS of optimal and OD cuprates[15] in that (i) the peak intensity increases with decreasing T and saturates [third to seventh lines from the bottom of Fig. 1(a)]. (ii) The peak frequency shifts from $0.30t$ (at $T = 0.1t$) to smaller values and saturates near $0.26t$ (at $T = 0.01t$). Note that this behavior is predicted in the heavily UD regime (doping $p \sim 0.04$). (iii) The low-frequency dependence at low T in clean systems varies as ω^a, with $a \approx 3.3$ for $T = 0.01t$, which resembles the cubic behavior of the low-frequency Raman response of B_{1g} in the superconducting state of OD and optimally doped cuprates.[3,4] As T increases, the ω^a law is replaced by a linear law, yielding a change reminescent of the one occurring in the superconducting state with increasing impurity scattering.[33] In Fig. 1(a) we show χ''_{B1g} at $T = 0.01t$ with static impurity scattering ($\eta = 0.5t$ and t; $\Gamma = \eta + \lambda\pi x$). The peak in B_{1g} loses weight then disappears, and the ω^a law is replaced by a linear one when η increases (compare solid curve, $\eta = 0$, with two lowest ones). So, in order to observe the PG peak in the B_{1g} response, samples will have to be clean ($\eta \rightarrow 0$).

Although a PG-induced peak was reported[34–36] at 600 cm^{-1} in UD Bi2212, it was later[37] shown to be a phonon peak created by oxygen disorder. The theoretical results here suggest the formation of a peak near a frequency of $\sim$240 cm^{-1} (in cuprates with a doping of 0.1 at room temperature) which falls in the same frequency range of a B_{1g} phonon mode found in Bi2212. Thus, it would be difficult to extract the behavior of this feature experimentally in Bi2212, and one would have to turn to the other families of cuprates to find this PG signature.

Figures 2(a)–2(d) show χ''_{B1g} and χ''_{B2g} versus ω for differ-

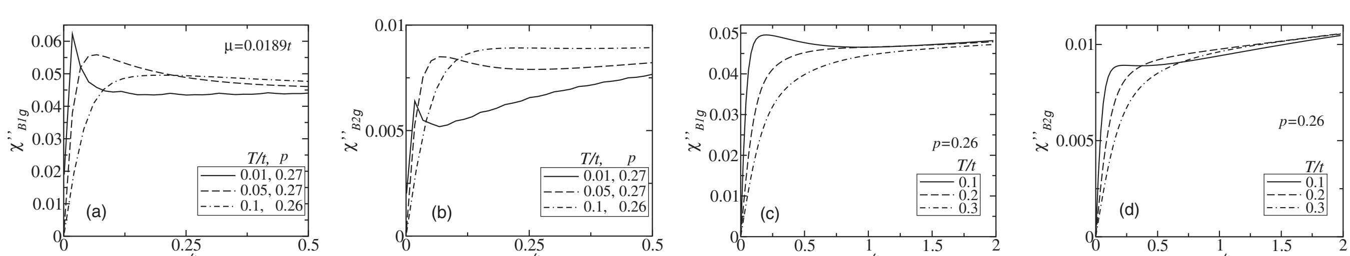

FIG. 2. The frequency dependence of χ''_{B1g} for (a) $0.01 \leq T/t \leq 0.1$ and (c) $0.1 \leq T/t \leq 0.3$; and of χ''_{B2g} for (b) $0.01 \leq T/t \leq 0.1$ and (d) $0.1 \leq T/t \leq 0.3$ are displayed for OD cuprates ($p \approx 0.26-0.27$). Here, $\mu \approx 0.019t$.

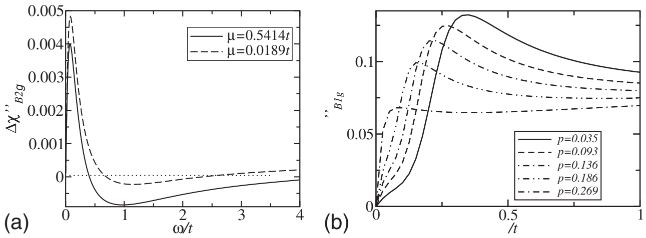

FIG. 3. (a) $\Delta\chi''_{B2g}=\chi''_{B2g}(T=0.1t)-\chi''_{B2g}(T=0.3t)$ in the UD (solid line) and OD (long-dashed line) regimes. (b) The doping dependence of the χ''_{B1g} peak is shown at $T=0.05t$.

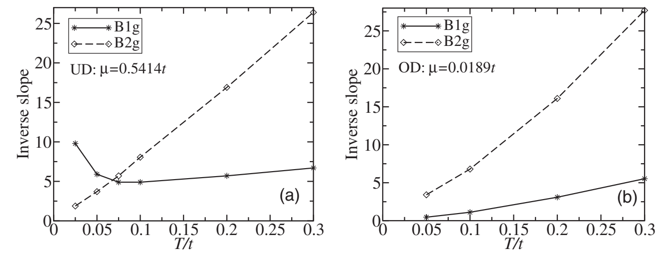

FIG. 4. The Raman relaxation rates for B_{1g} and B_{2g} are plotted vs temperature in the (a) UD and (b) OD regimes.

ent temperatures in the OD regime with $p\approx0.26$. Note that in B_{1g} there is a change in the frequency dependence of low-ω scattering with doping; in the OD cuprates, the response is linear in frequency, but is near cubic in the UD regime. This change takes place at optimal doping. In the OD regime, the frequency and the temperature trends for χ''_{B1g} and χ''_{B2g} compare well to experimental data.[19]

When comparing B_{2g} spectra at $T=0.3t\approx300$ K and $0.1t\approx100$ K in Figs. 1(b) and 1(d), it is evident that spectral weight is lost at higher frequencies and gained at lower ones as T decreases. This B_{2g} spectral weight redistribution $[\Delta\chi''_{B2g}=\chi''_{B2g}(T=0.1t)-\chi''_{B2g}(T=0.3t)]$ is presented more clearly in Fig. 3(a), where a crossover is found at $\omega=0.35t\approx280$ cm^{-1} in the UD ($\mu=0.5414t$) regime, and at $\omega\approx600$ cm^{-1} in the OD ($\mu=0.0189t$) cuprate. Integration of $\Delta\chi''_{B2g}$ between $\omega=0$ and $\omega=5t$ gives (approximately) 1.4×10^{-3} in this OD regime and -9.3×10^{-4} in the UD one. Note that doping is almost T independent in the OD regime ($p\approx0.26$), but decreases with T in the UD regime from $p\approx0.1$ ($T=0.3t$) to $p\approx0.04$ ($T=0.1t$) (see Ref. 26 for the T dependence of doping in RAFT). Opel *et al.*[6] found a depletion of spectral weight below ≈800 cm^{-1}, but no enhancement of weight at lower frequencies. However, their raw spectra show an enhancement at lower frequencies with which our result [Fig. 3(a)] is in agreement. Note that the results reported in Fig. 1(d) with $\eta=0$ or those in Fig. 1(b) with $\eta>0$ are consistent with experimental data; with decreasing T, spectral weight transfers from higher frequencies to lower ones, and the slope at zero ω increases, as found by Nemetschek *et al.*[38] It seems, thus, that the PG signature in Raman is characterized by a T-dependent crossover in B_{2g} and a peak in B_{1g}.

Another signature of the PG in Raman experiments is the doping dependent changes in the B_{1g} response, which strongly decreases with underdoping into the PG state. For $La_{2-x}Sr_xCuO_4$, the ratio of the integrated intensity (in the range of frequencies $0\leq\omega\leq600$ cm^{-1}) of χ''_{B1g} to χ''_{B2g} decreases gradually from 5 in the OD regime ($x=0.22$) and then more rapidly below optimal to <1 in the UD regime ($x=0.10$).[13] The present model does not recover this result because we do not yet have access to a self-energy derived from first principles—a difficult problem which is presently being pursued. With underdoping away from the optimal point in the clean limit, the position (frequency) of the peak in B_{1g} is found to increase, Fig. 3(b). This doping dependence mimics the doping dependence of the PG onset temperature T^*, not that of the superconducting T_c. We believe that self-energy effects will affect both the peak position and its weight, so it remains to be seen whether the doping-dependent suppression of χ''_{B1g} will be reproduced.

Figures 4(a) and 4(b) show the Raman relaxation rates $\Gamma_i=[d\chi''_i/d\omega|_{\omega=0}]^{-1}$ versus T. For B_{2g}, Γ_{B2g} is linear in T in both the UD and OD regimes, implying that the cold electrons near the points $(\pm\frac{\pi}{2},\pm\frac{\pi}{2})$ display a metallic behavior. Γ_{B1g} is T independent at high temperature, but increases as T decreases in the UD regime; while it decreases linearly with T in the OD regime. The hot electrons therefore show an insulatinglike behavior at low T in the UD regime, and a metalliclike behavior in the OD regime. A metal-insulator transition seems to take place in the vicinity of optimal doping, in agreement with the dichotomy of the cold and hot electrons found in experiment.[6,10,18] Opel *et al.*[6] found that the static scattering rate extracted in the UD regime using their Raman data increases with decreasing temperature, a result which was said to contradict the MFL behavior of the static (i.e., $\omega=0$) scattering rate. However, we find that a MFL self-energy reproduces the behavior found by Opel *et al.*

We also examined the dependence of the slopes Γ_i^{-1} on the scattering rate η at low temperature and found a scaling crossover at $\eta\sim t$. Figure 5 displays this slope versus η for $U=2.8t$, $t'=-0.16t$, and $T=0.01t$. Both slopes are characterized by two regimes: they behave as $1/\eta$, which is consistent with a Drude-type behavior, in the low scattering limit ($\eta/t\ll1$), but as $1/\eta^2$ in the strong scattering limit ($\eta/t\gg1$). So the idea that the resistivity in a Drude-type scenario[6] can be deduced from the slopes of the Raman response is inaccurate in the dirty limit according to the present finding.

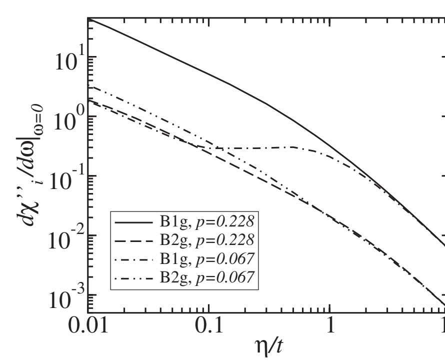

FIG. 5. The slope $d\chi''_i(\omega)/d\omega|_{\omega=0}$ with $i=B_{1g}$ or B_{2g} is plotted versus η/t on a log-log scale. For comparison purposes, curves for the UD ($p=0.067$) and OD ($p=0.228$) states are plotted together.

IV. CONCLUSION

To conclude, RAFT is used to analyze the normal-state Raman response in the high-T_c cuprates. This theory predicts a PG-induced peak in the B_{1g} response in the clean limit and recovers the B_{1g}-B_{2g} dichotomy. While it is beyond the scope of this paper, it remains to be seen what changes are predicted to occur upon entering the superconducting state where another remarkable dichotomy exists in the B_{1g} vs B_{2g} response. At the transition to the superconducting state a pair-breaking peak is induced in B_{2g}, but no discernable changes are observed in B_{1g}. In addition, the integrated spectral weight ratio (of B_{1g} to B_{2g}) is suppressed with underdoping. Although some progress has been made in Ref. 29, where the MFL self-energy effects were ignored and a temperature-independent PG has been used (in our case the PG is T dependent), the resolution of these two long-standing issues in the field of ERS requires further theoretical analysis.

ACKNOWLEDGMENTS

M.A. acknowledges the financial support of the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Laurentian University Research Fund, and Dalhousie University for his visits. K.H. acknowledges the support of NSERC and the Dalhousie Institute for Research in Materials, and Laurentian University for his visits.

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