Resonant Raman scattering from a spin density wave insulator

A. P. Kampf¹ and W. Brenig²

¹ Institut für Festkörperforschung, Forschungszentrum Jülich, Postfach 1913, W-5170 Jülich, Germany
 ² Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, W-5000 Köln 41, Germany

Abstract. We present a calculation of the electronic Raman cross section for the scattering of light across the energy gap of an antiferromagnetic insulator. The antiferromagnet is described in terms of a spin density wave state for the Hubbard model at half filling. We consider the coupling of the light to the current density and the inverse mass tensor on equal footing. A comparison of the cross section for different scattering geometries is given.

Keywords: Spin density waves; Raman scattering; High temperature superconductors.

1 Introduction

Experimental and theoretical studies of Raman light scattering in antiferromagnets have commonly focused on the two-magnon contribution to the intensity of the scattered light. In particular the investigation of the antiferromagnetic parent compounds of the high temperature superconductors has renewed the interest in this field. The magnetic properties of undoped La₂CuO₄ are well described by a two-dimensional antiferromagnetic spin 1/2 Heisenberg model for the magnetic moments of the Cu²⁺ ions [1]. The in-plane quantum spin excitations give rise to a broad two-magnon peak at around 3000 cm⁻¹ in the Raman spectrum [2]. The understanding of the position and the lineshape has been shown to require approaches beyond spin wave theory which include quantum effects and magnon-magnon interactions [3].

In an itinerant magnetic system, and in contrast to the above mentioned scattering of light from the collective degrees of freedom, there are additional single particle effects which have received less attention in the literature. Thus, in this note we focus on the purely electronic contribution to the Raman intensity which arises from resonant scattering across the energy gap of an itinerant antiferromagnetic (AF) insulator. In the cuprate materials this energy gap is related to the spin density wave (SDW) gap which is obtained at half filling for the effective single band Hubbard model, which results from the well known transformation [4] of the three band model for the direct overlap of Cu and O orbitals, onto a one band model. In the following we therefore describe the magnetic system in terms of an SDW state in a single band Hubbard model at half filling. If RPA fluctuations around the mean field static SDW are included this approach has been shown to reproduce the results of linear spin wave theory in the limit of a large on site Coulomb repulsion of the itinerant electrons [5]. Needless to say, the extension to the metallic regime away from half filling is of particular interest and relevance to the high temperature superconductors. Their normal state Raman response function is highly unusual and shows an almost featureless continuum ranging from thermal up to energies on the 1 eV scale which cannot be explained by standard two-phonon contributions and is likely to be electronic in origin [6].

Despite all theoretical efforts to describe the normal state properties of high temperature superconductors in terms of strongly interacting electron models only a limited number of works have addressed the problem of Raman light scattering from correlated systems. As yet another first step into this direction we will calculate the relevant response function in the simple limit of a half filled single band Hubbard model. We will discuss the possible extension of our approach to include two-magnon scattering and to the doped AF correlated metal regime at the end of our paper.

2 Electronic Raman scattering

Shastry and Shraiman have recently outlined a theory for Raman scattering in Mott-Hubbard systems [7]. Based on their approach we start from the Hubbard Hamiltonian on a square lattice in the presence of an external transverse electromagnetic photon field represented by the vector potential A

$$H_{\mathbf{A}} = -t \sum_{\langle ij \rangle, \sigma} \left[e^{j \frac{e}{c} \int_{i}^{j} \mathbf{A} \cdot \mathbf{dl}} c_{i\sigma}^{\dagger} c_{j\sigma} + h. c. \right] + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$
(1)

where as usual $c_{i\sigma}^+(c_{i\sigma})$ destroys (creates) an electron of spin σ on the site *i* of the lattice and the sum on $\langle ij \rangle$ is restricted to next nearest neighbors. *t* and *U* represent the hopping integral and the on-site Coulomb repulsion, respectively, and $n_{i\sigma}$ is the local density. We expand to second order in **A** and in performing the Fourier transformation we introduce the components of the current operator

$$j_{\mathbf{q}}^{a} = \sum_{\mathbf{k}\sigma} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_{a}} c_{\mathbf{k}+\mathbf{q}/2,\sigma}^{+} c_{\mathbf{k}-\mathbf{q}/2,\sigma}$$
(2)

and the components of the inverse mass tensor

$$\tau_{\mathbf{q}}^{\alpha\beta} = \sum_{\mathbf{k}\sigma} \frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_{\alpha} \partial k_{\beta}} c_{\mathbf{k}+\mathbf{q}/2,\sigma}^+ c_{\mathbf{k}-\mathbf{q}/2,\sigma}$$
(3)

with the tight binding dispersion $\varepsilon_{\mathbf{k}} = -2t(\cos(k_x a) + \cos(k_y a))$. Only for a free electron dispersion is $\tau_{\mathbf{q}}^{\alpha\beta}$ proportional to the familiar density operator. With this notation we obtain the effective Hamiltonian

$$H_{\mathbf{A}} = H_{\mathbf{A}=0} - \frac{e}{c} \sum_{\mathbf{q}\alpha} j^{\alpha}_{\mathbf{q}} A^{\alpha}_{-\mathbf{q}} + \frac{1}{2} \left(\frac{e}{c}\right)^{2} \sum_{\mathbf{q},\mathbf{q}_{2}\alpha\beta} \tau^{\alpha\beta}_{\mathbf{q}_{1}+\mathbf{q}_{2}} A^{\alpha}_{-\mathbf{q}_{1}} A^{\beta}_{-\mathbf{q}_{2}}$$
(4)

We write the components of the electromagnetic field operator A^{a} in the second quantized form as

$$A_{\mathbf{q}}^{a} = \sqrt{\frac{hc^{2}}{\Omega_{\mathbf{q}}\omega}} (e_{a} a_{-\mathbf{q}} + \bar{e}_{a} a_{\mathbf{q}}^{+})$$
(5)

where e_a are the complex components of the unit vector **e** of the photon polarisation and the overbar denotes complex conjugation, $\omega_q = c |\mathbf{q}|$ is the photon energy and $a_q^+(a_q)$ are the photon creation (annihilation) operators, respectively.

The Raman scattering cross section is proportional to the transition rate R which can be obtained by applying Fermi's Golden Rule. The inelastic scattering rate for transitions with energy and momentum transfer $\omega = \omega_f - \omega_i$ and $\mathbf{q} = \mathbf{k_f} - \mathbf{k_i}$ is therefore of the form

$$R(\mathbf{q},\,\omega) = \frac{hc^2}{\Omega\,\sqrt{\omega_i\omega_f}} \left(\frac{e}{c}\right)^4 \sum_{i,f} \frac{e^{-\beta\varepsilon_i}}{Z} |\langle f \mid \hat{M} \mid i \rangle |^2 \,\delta(\varepsilon_f - \varepsilon_i - \omega) \qquad (6)$$

where Z is the partition function and $\beta = 1/k_B T$ is the inverse temperature. \hat{M} is the effective scattering operator responsible for transitions between initial and final eigenstates of the Hubbard Hamiltonian with energy eigenvalues ε_i and ε_f , respectively. From the electron-light coupling Eq. (4) there are two contributions to \hat{M} , a direct scattering from the coupling to the inverse mass tensor and a resonant contribution from the coupling to the current, which involves virtual intermediate states. Explicitly, one finds

$$\langle f \mid \hat{M} \mid i \rangle = \sum_{\alpha\beta} e_i^{\alpha} \bar{e}_j^{\beta} \left\langle f \mid \frac{1}{2} \tau_{\mathbf{q}}^{\alpha\beta} + \hat{M}_R^{\alpha\beta} \mid i \right\rangle$$
 (7a)

$$\langle f \mid \hat{M}_{R}^{a\beta} \mid i \rangle = \sum_{\nu} \left[\frac{\langle f \mid j_{\mathbf{k}_{t}}^{\beta} \mid \nu \rangle \langle \nu \mid j_{-\mathbf{k}_{i}}^{a} \mid i \rangle}{\varepsilon_{\nu} - \varepsilon_{i} - \omega_{i}} + \frac{\langle f \mid j_{-\mathbf{k}_{i}}^{a} \mid \nu \rangle \langle \nu \mid j_{\mathbf{k}_{t}}^{\beta} \mid i \rangle}{\varepsilon_{\nu} - \varepsilon_{i} + \omega_{f}} \right]$$
(7b)

where the two terms for the resonant scattering operator arise from two different time orderings. Using the fluctuation dissipation theorem it is useful to rewrite the transition rate in terms of the imaginary part of a corresponding dynamical susceptibility.

$$R(\mathbf{q},\,\omega) = \left[1 + n(\omega)\right] \frac{1}{2\pi} \frac{hc^2}{\Omega \sqrt{\omega_i \omega_f}} \left(\frac{e}{c}\right)^4 \int dt e^{-i\omega t} \left\langle \left[\hat{M}^+(0),\,\hat{M}(t)\right] \right\rangle \tag{8}$$

Here $n(\omega)$ is the Bose distribution function, but in what follows we will only consider the limit of zero temperature $T \rightarrow 0$. The scattering operator is given by

$$\hat{M}(t) = \sum_{\alpha\beta} e_i^{\alpha} \bar{e}_f^{\beta} \left(\frac{1}{2} \tau_{\mathbf{q}}^{\alpha\beta}(t) + i \int_{0}^{\infty} dt' \left[j_{-\mathbf{k}_i}^{\alpha}(t+t'), j_{\mathbf{k}_i}^{\beta}(t) \right] e^{-i\omega_i t'} \right)$$
(9)

The time dependence of $\hat{M}(t) = e^{itH_{\Lambda^{-0}}} \hat{M} e^{-itH_{\Lambda^{-0}}}$ is determined by the Hubbard Hamiltonian in the absence of the photon field. Since the wavelength of light in the optical range is large compared to the lattice spacing and all length scales of the electronic system, we can safely neglect the momentum transfer of the photon and we will from now

on use $\mathbf{q} = \mathbf{k}_{\mathbf{f}} - \mathbf{k}_{\mathbf{i}} = 0$. We refer the reader to the work of Shastry and Shraiman [7] for a more complete exposition of the formal manipulations outlined above. Note that their derivation did not rely on any specific form of the electron-electron interaction since the photon field couples to the electrons only through the phase factor in the kinetic energy.

3 Raman scattering from a spin density wave insulator

In this section we apply Eq. (8, 9) to study the Raman scattering from the Hubbard model for the special case of half filling. As mentioned earlier an explicit calculation is feasible in this case since here long range antiferromagnetism is well established (at least at T =0 in two dimensions) and we may use the mean field weak coupling SDW formalism to describe the broken symmetry state. The Hartree-Fock factorized Hamiltonian is diagonalized by the Bogoliubov transformation [5]

$$\gamma_{\mathbf{k},\sigma}^{\nu} = u_{\mathbf{k}} c_{\mathbf{k},\sigma} + v_{\mathbf{k}} \sigma c_{\mathbf{k}+\mathbf{Q},\sigma}$$

$$\gamma_{\mathbf{k},\sigma}^{\nu} = v_{\mathbf{k}} c_{\mathbf{k},\sigma} - u_{\mathbf{k}} \sigma c_{\mathbf{k}+\mathbf{Q},\sigma}$$
(10)

mixing the bare electron states $|\mathbf{k}\rangle$ and $|\mathbf{k} + \mathbf{Q}\rangle$ due to Bragg scattering from the commensurate AF spin order. $\mathbf{Q} = (\pi, \pi)$ is the AF wavevector and v_k and v_k are the standard coherence factors

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2} \left(1 + \frac{\varepsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} \right)} \qquad v_{\mathbf{k}} = \sqrt{\frac{1}{2} \left(1 - \frac{\varepsilon_{\mathbf{k}}^2}{E_{\mathbf{k}}^2} \right)}$$
(11)

The tight binding band is split into a valence and a conduction band separated by twice the SDW energy gap $2\Delta_{SDW}$. The diagonalized Hamiltonian is then given by

$$H = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} (\gamma_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c} - \gamma_{\mathbf{k},\sigma}^{\nu+} \gamma_{\mathbf{k},\sigma}^{\nu})$$
(12)

with $E_k = \sqrt{\varepsilon_k^2 + \Delta_{SDW}^2}$ and due to the doubling of the unit cell the momentum sum is restricted to the magnetic Brillouin zone (MBZ) as indicated by the primed sum. In this Hartree-Fock state the time dependence of the bare electron operators is determined by Eq. (10) and

$$\gamma_{\mathbf{k},\sigma}^{c}(t) = \gamma_{\mathbf{k},\sigma}^{c} e^{-itE_{\mathbf{k}}} \qquad \gamma_{\mathbf{k},\sigma}^{v}(t) = \gamma_{\mathbf{k},\sigma}^{v} e^{itE_{\mathbf{k}}}$$
(13)

for momenta $\mathbf{k} \in MBZ$. Since we have discarded residual quasiparticle interactions within the Hartree-Fock Hamiltonian Eq. (12) we now may obtain an explicit form for the Raman scattering operator Eq. (9) whereby the light couples only the effective single particle excitations of the SDW state. After straightforward calculation we find

$$\tau_{\mathbf{q}=0}^{a\beta}(t) = 2 \sum_{\mathbf{k}\sigma}^{\prime} \frac{\partial^{2} \varepsilon_{\mathbf{k}}}{\partial k_{a} \partial k_{\beta}} \left(u_{\mathbf{k}}^{2} \gamma_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c} + u_{\mathbf{k}} v_{\mathbf{k}} \gamma_{\mathbf{k},\sigma}^{c+}(t) \gamma_{\mathbf{k},\sigma}^{v}(t) + v_{\mathbf{k}} v_{\mathbf{k},\sigma}^{c+}(t) \gamma_{\mathbf{k},\sigma}^{v}(t) + v_{\mathbf{k}} v_{\mathbf{k},\sigma}^{c+}(t) \gamma_{\mathbf{k},\sigma}^{v}(t) + v_{\mathbf{k}}^{2} \gamma_{\mathbf{k},\sigma}^{v+} \gamma_{\mathbf{k},\sigma}^{v} \right)$$

$$M_{R}^{a\beta}(t) = 4 \sum_{\mathbf{k}\sigma}^{\prime} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_{a}} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_{\beta}} u_{\mathbf{k}} v_{\mathbf{k}} \left(u_{\mathbf{k}} v_{\mathbf{k}} m_{\mathbf{k}}^{cc} \gamma_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c} + v_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c+} + v_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c+} + v_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c+} + v_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c+} \gamma_{\mathbf{k},\sigma}^{c+} + v_{\mathbf{k},\sigma}^{c+} + v_{\mathbf{k},\sigma}$$

$$(u_{\mathbf{k}}^{2} - v_{\mathbf{k}}^{2}) m_{\mathbf{k}}^{cv} \gamma_{\mathbf{k},\sigma}^{c+}(t) \gamma_{\mathbf{k},\sigma}^{v}(t) + (u_{\mathbf{k}}^{2} - v_{\mathbf{k}}^{2}) m_{\mathbf{k}}^{vc} \gamma_{\mathbf{k},\sigma}^{v+}(t) \gamma_{\mathbf{k},\sigma}^{c}(t) + u_{\mathbf{k}} v_{\mathbf{k}} m_{\mathbf{k}}^{vv} \gamma_{\mathbf{k},\sigma}^{v+} \gamma_{\mathbf{k},\sigma}^{v})$$
(14b)

Here we have introduced the following abbreviations to represent the various energy denominators for the different scattering processes between the valence and the conduction band

$$m_{\mathbf{k}}^{cc} = -m_{\mathbf{k}}^{vv} = \frac{1}{\omega_i - 2E_{\mathbf{k}} - i\delta} - \frac{1}{E_{\mathbf{k}}}$$
 (15a)

$$m_{\mathbf{k}}^{cv} = \frac{1}{\omega_i} - \frac{1}{\omega_i - 2E_{\mathbf{k}} - i\delta} \quad m_{\mathbf{k}}^{vc} = \frac{1}{\omega_i + 2E_{\mathbf{k}} - i\delta} - \frac{1}{\omega_i}$$
(15b)

For the remaining calculation of the scattering response function four commutators need to be evaluated corresponding to the different diagrams shown in Fig. 1 [8]. At half filling the insulating gap allows only for interband transitions between the valence and the conduction band to contribute to the scattering intensity. Since we assume that $k_BT \ll 2\Delta_{\text{SDW}}$ we list the different contributions for T = 0.



$$R(\mathbf{q} = 0, \omega) = \frac{1}{2} \frac{hc^2}{\Omega \sqrt{\omega_i \omega_f}} \left(\frac{e}{c}\right)^4 \left[R_{\tau\tau} + R_{\tau R} + R_{R\tau} + R_{RR}\right]$$
(16a)

$$R_{\tau\tau} = \sum_{\mathbf{k}\sigma} P_{\tau\tau}(\mathbf{k}) u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 \pi \left[\delta(\omega - 2E_{\mathbf{k}}) - \delta(\omega + 2E_{\mathbf{k}}) \right]$$
(16b)

$$R_{\tau R} + R_{R\tau} = -\sum_{k\sigma} P_{R\tau}(k) 4u_{k}^{2} v_{k}^{2} (u_{k}^{2} - v_{k}^{2}) 2\pi \times [2Re(m_{k}^{vc}) \delta(\omega - 2E_{k}) - 2Re(m_{k}^{cv}) \delta(\omega + 2E_{k})]$$

$$R_{RR} = 2\sum_{k\sigma} P_{RR}(k) 4u_{k}^{2} v_{k}^{2} (u_{k}^{2} - v_{k}^{2})^{2} 2\pi \times [|m_{k}^{vc}|^{2} \delta(\omega - 2E_{k}) - |m_{k}^{cv}|^{2} \delta(\omega + 2E_{k})]$$
(16c)
(

This result for the scattering intensity is naturally restricted to photon frequency shifts $\omega < \omega_i$. The different combinations of the polarisations of the incoming and outgoing photons are absorbed into the symmetry coefficients $P_{\tau\tau}$, $P_{R\tau}$, and P_{RR} . They are given by

$$P_{\tau\tau}(\mathbf{k}) = \sum_{a\beta\gamma\delta} e_i^a \, \bar{e}_f^\beta \, \frac{\partial^2 \, \varepsilon_{\mathbf{k}}}{\partial k_a \, \partial k_\beta} \, e_i^\gamma \, \bar{e}_f^\delta \, \frac{\partial^2 \, \varepsilon_{\mathbf{k}}}{\partial k_\gamma \, \partial k_\delta}$$

$$P_{R\tau}(\mathbf{k}) = \sum_{a\beta\gamma\delta} e_i^a \, \bar{e}_f^\beta \, \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_a} \, \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\beta} \, e_i^\gamma \, \bar{e}_f^\delta \, \frac{\partial^2 \, \varepsilon_{\mathbf{k}}}{\partial k_\gamma \, \partial k_\delta}$$

$$P_{RR}(\mathbf{k}) = \sum_{a\beta\gamma\delta} e_i^a \, \bar{e}_f^\beta \, \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_a} \, \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\beta} \, e_i^\gamma \, \bar{e}_f^\delta \, \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\beta} \, \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\beta}$$
(17)

The polarisation vectors of the photons for different scattering geometries are collected in Table 1 and the corresponding symmetry coefficients in Table 2. The energy conserving δ -functions in Eq. 16 appear as in a conventional Golden Rule analysis for light induced transitions. The absorption sets in when the incoming photon energy exceeds $2\Delta_{SDW}$ and the spectral weight of the transition is determined by matrix elements which appear in the form of different coherence factor combinations of the underlying spin density wave.

Table 1 Scattering geometries for different combinations of the polarisation vectors of the incoming and outgoing photons \mathbf{e}_i and \mathbf{e}_f , respectively

| Symmetry | ei | e _f |
|-------------------------------|-----------------------------|-----------------------------|
| A_{1g} | $\frac{1}{\sqrt{2}}(1, 1)$ | $\frac{1}{\sqrt{2}}(1, 1)$ |
| <i>B</i> _{1g} | $\frac{1}{\sqrt{2}}$ (1, 1) | $\frac{1}{\sqrt{2}}(1, -1)$ |
| <i>B</i> _{2<i>g</i>} | (1, 0) | (0, 1) |

It is generally known for nearly free electron systems that the photons are dominantly scattered by density fluctuations [9] and the coupling to current fluctuations is usually neglected [10]. These arguments are based on the experimentally common situation that the optical energies are large compared to important electronic excitation energies. In

| $P_{R\tau}$ | | P_{RR} |
|---|---|---|
| $\frac{sk_{x} + \cos k_{y}}{sk_{x} - \cos k_{y}}^{2} = \frac{2t^{3}(s)}{2t^{3}(s)}$ | $n k_x + \sin k_y)^2 (\cos k_x + \cos k_y)$ $n k_x^2 - \sin k_y^2) (\cos k_x - \cos k_y)$ | $4t^{4}(\sin k_{x} + \sin k_{y})^{4}$ $4t^{4}(\sin k_{x}^{2} - \sin k_{y}^{2})^{2}$ $4(t^{4} \sin k_{x}^{2} - \sin k_{y}^{2})^{2}$ |
|)) | $\frac{P_{R\tau}}{\cos k_x + \cos k_y)^2} = 2t^3 (\sin \theta)^2$ $\cos k_x - \cos k_y)^2 = 2t^3 (\sin \theta)^2$ | $\frac{P_{R\tau}}{\cos k_x + \cos k_y)^2} = \frac{2t^3 (\sin k_x + \sin k_y)^2 (\cos k_x + \cos k_y)}{2t^3 (\sin k_x^2 - \sin k_y^2) (\cos k_x - \cos k_y)}$ 0 |

Table 2 Symmetry coefficients $P_{\tau\tau}$, $P_{R\tau}$, and P_{RR} for different scattering geometries

addition, possible cancellation effects of the two time ordered contributions of the $\mathbf{j} \cdot \mathbf{A}$ coupling in Eq. (7b) may cause a further reduction in magnitude. In the case of resonant scattering from a spin density wave insulator, however, the situation is more subtle. On the one hand the $\mathbf{j} \cdot \mathbf{A}$ contributions are reduced in magnitude since they appear with higher power in the coherence factors due to the second order of the resonant scattering part R_{RR} . On the other hand they are strongly enhanced if the energy of the incoming photon is near $2\Delta_{\text{SDW}}$ or in general, if the Raman frequency shift becomes comparable to the incoming photon energy. This effect is represented by the prefactors m^{cv} and m^{vc} .

Apart from the above variation of the Raman cross section as a function of frequency there is an additional dependence of the scattering intensity on the various polarisation geometries. In Fig. 2(a) and Fig. 2(b) we show the results of a numerical evaluation of Eq. (16a) for the Raman transition rate for two particular scattering geometries namely B_{1g} and A_{1g} , respectively, at fixed ω_i . For B_{1g} symmetry a strong peak appears near the threshold energy $2\Delta_{\text{SDW}}$ which arises from the coupling to the inverse mass tensor (i. e. density) fluctuations alone. As evident from Fig. 2(b) this peak, however, is entirely wiped out for A_{1g} symmetry where $P_{\tau\tau} = 1/4 \varepsilon_k^2$ which vanishes near the top of the valence band for the transitions with $\omega = 2\Delta_{\text{SDW}}$. A similar argument applies for B_{2g} scattering, where the symmetry factor $P_{\tau\tau}$ is identically zero. These symmetry features may help to identify a SDW gap in a Raman scattering experiment. As a generic feature it is seen from Fig. 2(a), (b) that the transition rate is enhanced with increasing photon frequency shift for the contributions from the coupling to the current fluctuations. Note in passing that even though the transition rate is a strictly nonnegative number the mixed term $(R\tau + \tau R)$ can be of either sign, as seen in comparing Fig. 2(a) and Fig. 2(b) for



Fig. 2 Contributions to the Raman scattering rate for (a) B_{1g} and (b) A_{1g} and symmetry for the different scattering processes of Fig. 1. Energies are in units of t

 B_{1g} and A_{1g} symmetry, respectively. We point out that for B_{2g} symmetry it is only R_{RR} which is finite.

With the parameters chosen as in Fig. 2 the energy of the incoming photon ω_i is well above the SDW gap energy. It is evident, that a variation of this frequency will lead to an additional truly resonant feature which is a consequence of the factors $m_k^{vc, cc, vv}$ as given in Eq. (15). If ω_i approaches $2\Delta_{\text{SDW}}$, a huge enhancement appears in each scattering geometry which can be traced back entirely to the **j** · **A** coupling.

To conclude our analysis, we discuss possible extensions of this work. A natural question besides the resonant features of the Raman scattering across the insulating gap of the antiferromagnet regards two-magnon excitations which would provide for a continuous low frequency contribution. In order to describe these spin-waves within our approach to the Hubbard model the fluctuations around the mean-field spin density wave ground state have to be included. This is most conveniently done using RPA for the transverse spin fluctuations in the two-band system of the SDW insulator [5]. Despite the general validity of our commutator analysis a standard diagrammatic approach may prove to be more convenient for evaluating the two-magnon scattering contribution to the Golden Rule.

Another issue of special interest involves the extension fo finite doping concentrations $\langle n_i \rangle = 1 - \delta < 1$ away from half-filling. Starting from the mean-field SDW ground state, a rigid band picture would allow the same analysis as we applied above. This picture is based on the assumption that for small doping concentrations the long range ordered SDW is still a valid starting point, and doped holes simply start to fill the top of the valence band. Particle-hole intra valence band transitions will then lead to Raman intensity below the gap energy. However, an analysis that includes only finite range magnetic correlations in the doped paramagnetic metal should be more appropriate. On the RPA level one may still evaluate the two-spin fluctuation Raman scattering analogously to the two-magnon scattering in the ordered antiferromagnet. We will present the results of a more complete diagrammatic analysis of the RPA extensions in a future note.

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