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Optical and Raman spectrum in the magnetic state of iron pnictides

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One of the big puzzles in iron-pnictides is to understand the unexpected anisotropy in the magnetic state between x and y direction seen in resistivity and optical conductivity[1] among other techniques. Raman experiments[2] have also seen a symmetry dependence of the arsenide phonon intensity indicating a strong in-plane anisotropy in the magnetic state. There is a strong debate about whether this anisotropy is driven by magnetism or by orbital ordering. Both degrees of freedom are coupled and difficult to disentangle. We consider a 5 orbital tight-binding model[3] at the Hartree-Fock level and calculate the Drude weight, the optical conductivity and the Raman response. Our results point against orbital ordering as the origin of the anisotropy in the Drude weight which may be ascribed to the anisotropy of the Fermi velocity for small magnetic moment[4]. We compare the orbital conductivity anisotropy with the frequency dependent orbital reorganization and find that the anisotropy is mostly magnetic in origin. We study the reorganization of the spectral weight in the optical and Raman spectrum upon varying the Hubbard interaction and the Hund's coupling. We also study the Raman response of the coupling of the arsenide optical phonon with the electronic continuum and compare with Raman experiments.[5]

[1] J.-H. Chu et al., Science 329, 824 (2010); Dusza et al, EPL 93 37002 (2011)
[2] S. Sugai et al., arXiv:1010. 6151; L. Chauvière et al., Physical Review B 84, 104508 (2011)
[3] M.J. Calderon, B. Valenzuela, E. Bascones, Phys. Rev. B 80, 094531 (2009).
[4] B. Valenzuela, E. Bascones, M. J. Calderón, Phys. Rev. Lett. 105, 207202 (2010)
[5] N. García, B. Valenzuela, M. J. Calderón, E. Bascones, G. León, E. Cappelluti, S. Chiuchi, (in preparation)

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