



FIG. 8: Imaginary part of  $\chi_0(\mathbf{q}, \omega)$  (eV) decomposed into the intra- and inter-band contributions. Results are plotted along  $\Gamma - M - \Gamma$  direction. (a)  $h - h$ , (b)  $e - h$  and (c)  $e - e$  contributions.

#### IV. CONCLUSION

In summary, we report detailed calculations of the independent electron susceptibility of non-magnetic  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$  as a function of doping and of the atomic positions within the unit cell. Our results are based on accurate electronic structure calculations within density functional theory, and include matrix elements from full potential linearized augmented plane wave method. We account properly for Fermi surface related features through an accurate sampling of the Brillouin zone.

The static susceptibility is peaked around the zone center and at the nesting vector  $\mathbf{q}_N$  ( $M$  point), due to intra-band ( $e - e$  and  $h - h$ ) and inter-band transitions respectively, and is consistent with the observed stripe AFM ordering. However, the peak at  $M$ -point is not as pronounced as reported in calculations with approximate or no matrix elements. Upon doping, the peak at  $M$  evolves into a volcano-like structure consistent with the incommensurate magnetic spiral state predicted by first principle calculations. The intra- and inter-band analysis of the contributions to  $\chi_0(q, 0)$  shows an  $e$  versus  $h$  asymmetry which may relate to the multigap character suggested by experiments. Our results could serve as a first step towards the definition of an *ab-initio* effective electron-electron interaction, necessary to obtain the pairing potential in pnictides.

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