The Linear Optical Conductivity in $BaNiS_2$ and $BaCoS_2$: Effects of Correlations and Dirac states

R. P. S. M. Lobo
LPEM, ESPCI Paris, PSL Research University, CNRS, 10 rue Vauquelin, 75005 Paris, France
Sorbonne Université, LPEM, CNRS, 75005 Paris, France

Email: lobo@espci.fr

$BaCo_{1-x}Ni_xS_2$ sulfides are quasi 2D Mott materials. The cobalt end member – $BaCoS_2$ – is an almost insulating, antiferromagnetic, strongly correlated system. Its optical conductivity shows an unusual linear behavior over a large energy range that extends all the way to zero frequency, contradicting a proposed charge-transfer Mott insulator scenario. A linear optical conductivity is often associated to Dirac cones. However, in $BaCoS_2$, these cones are far from the Fermi level. Utilizing *ab initio* dynamical mean field theory, we show that the linear conductivity of $BaCoS_2$ originates from a non-Fermi liquid at the verge of a metal-insulator transition accompanied by an incipient opening of a charge-transfer gap and an incoherent charge transport driven by electronic correlations. Replacing Co by Ni leads to a metallic material with a strong coherent Drude peak. In $BaNiS_2$, the Dirac states get pushed close to the Fermi level. The DOS at the Fermi level is strongly temperature dependent and a Drude peak narrowing is accompanied by an unexpected spectral weight transfer to higher energies. We explain this transfer through a competition between Dirac and bulk states.

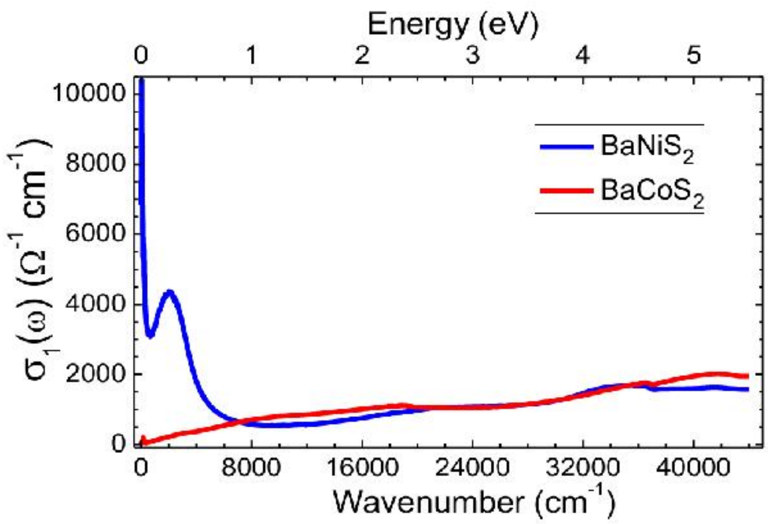

Figure. Optical conductivity of insulating $BaCoS_2$ and conducting $BaNiS_2$. The insulating material is close to a Mott transition and its low energy σ_1 is dominated by a linear response. The linear conductivity survives in the conducting material and competes with a Drude peak and contributions from a low density of states close to the Fermi level.

Collaborators: D. Santos-Cottin, M. Casula, Y. Klein, P. Werner, T. Miyake, L. de'Medici, and A. Gauzzi

References

[1] D. Santos-Cottin *et al.*, *Linear behavior of the optical conductivity and incoherent charge transport in $BaCoS_2$*, arXiv: 1712.01539