The Linear Optical Conductivity in BaNiS\textsubscript{2} and BaCoS\textsubscript{2}: Effects of Correlations and Dirac states

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BaCo\textsubscript{1-x}Ni\textsubscript{x}S\textsubscript{2} sulfides are quasi 2D Mott materials. The cobalt end member – BaCoS\textsubscript{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\textsubscript{2}, these cones are far from the Fermi level. Utilizing \textit{ab initio} dynamical mean field theory, we show that the linear conductivity of BaCoS\textsubscript{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\textsubscript{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.

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\textbf{References}