

# Landau Quantization in Coupled Weyl Points: a Case Study of Semimetal NbP

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### Introduction

Weyl semimetal (WSM) is a newly discovered quantum phase of matter that exhibits topologically protected states characterized by two separated Weyl points (WPs) with linear dispersion in all directions. However, in real-world WSMs the coupling between the WPs is inevitable, resulting in band hybridization when the linear bands from each WPs overlap (Fig.1a). The band hybridization leads to gap opening between the upper and lower conduction (or valence) bands as well as unique optical responses, particularly when a high magnetic field is applied. In this study, we combine the theoretical analysis and magneto-infrared spectroscopy of an archetypal Weyl semimetal, niobium phosphide (NbP), to quantitatively describe such coupling effects.

#### Experimental

Single crystals of NbP were prepared by chemical vapor transport technique using iodine as the transporting agent. The magneto-infrared (IR) reflectance measurements were carried out using standard Fourier-transform infrared spectroscopy technique at liquid helium temperature and in magnetic fields (*B*) up to 17.5 T in SCM3 of the DC Field Facility. All the measurements were performed in Faraday geometry with the magnetic field applied along the [001] direction of the sample.

#### **Results and Discussion**

Figure 1b shows the calculated magnetic field dispersion of the Landau level (LL) transitions in coupled WPs [1]. In contrast to the case of isolated WPs, where the interband LL transitions are solely Dirac-like and following a square-root magnetic field dependence, the transitions in coupled WPs exhibit additional spectroscopic features involving the upper (lower) conduction (valence) band as well as the magnetic field induced gap at the charge neutrality. The presence of the upper (lower) conduction (valence) band is due to the coupling induced band hybridization (Fig. 1a), which gives rise to the crossing/anticrossing behavior in the LL transition spectra (Fig. 1b). The gap opening at the charge neutrality, on the other hand, is manifested by a particular transition labeled as mode A in Fig. 1b. The magnetic field dispersion of this mode depends strongly on the field direction. When the magnetic field is applied perpendicular to the separation of the WPs (which breaks the axial symmetry of the system), it is also accompanied by a new optical transition rule for interband LL transitions. Overall, we find that all these behaviors can be quantitatively described by an effective Hamiltonian model for coupled WPs with a finite mass parameter. The robustness of the topologically protected Weyl states depends on the relation between the mass and the spin splitting in the material.

#### Conclusions

We have demonstrated both theoretically and experimentally the essential role of the coupling effect between WPs in

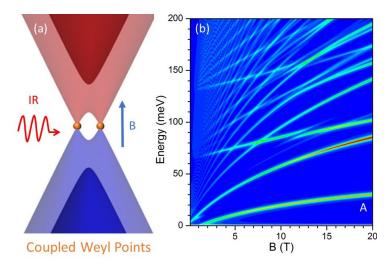
an established WSM, NbP. Our band structure analysis predicts several unique spectroscopic features originated from the CWPs that were largely confirmed in the magneto-spectroscopy experiment. These results emphasize the importance of coupling between WPs both for fundamental understanding of Weyl fermions in realistic condensed matter systems and for future device applications.

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#### References

[1] Jiang, Y. et al. Nano Lett., in press.



**Fig. 1.** (a) Band structure of coupled WPs at zero magnetic field. (b) Calculated LL transition spectra using the coupled WPs model [1].