Phonon-assisted luminescence in qubits from many-body perturbation theory

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Phonon-assisted luminescence is a key property of defect centers in semiconductors, and can be measured to perform the readout of the information stored in a quantum bit, or to detect temperature variations.
The investigation of phonon-assisted luminescence usually employs phenomenological models, such as that of Huang and Rhys, with restrictive assumptions that can fail to be predictive.
In this work, we predict luminescence and study exciton-phonon couplings within a rigorous many-body perturbation theory framework,
an analysis that has never been performed for defect centers.
In particular, we study the optical emission of the negatively-charged boron vacancy in 2D hexagonal boron nitride, which currently stands out among defect centers in 2D materials thanks to its promise for applications in quantum information and quantum sensing. We show that phonons are responsible for the observed luminescence, which otherwise would be dark due to symmetry. We also show that the symmetry breaking induced by the static Jahn-Teller effect is not able to describe the presence of the experimentally observed peak at 1.5 eV.

References

[1] F. Libbi. P. Melo, Z. Zanolli, M. J. Verstraete and N. Marzari, arXiv:2111.03518

Figures

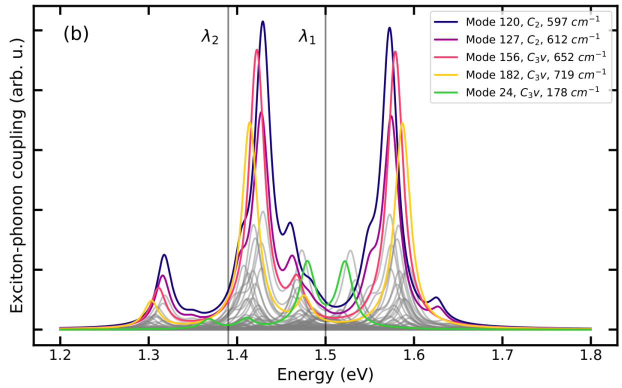

Figure 1: Exciton-phonon coupling function for the negatively charged boron vacancy in 2D hBN. The phonon modes which couple most strongly with excitons are enlightened with coloured lines and reported in the legend in decreasing order of contribution, while the other phonon modes are represented with grey lines.