Long tailed trions in MoS_2, and charge and screening signatures in graphene/hBN sandwiches

Jason Christopher[1], Xuanye Wang[2], Bennett Goldberg[1,2,3] and Anna Swan[2,1,3]

[1]*Physics Department Boston University 590 Commonwealth Avenue, Boston, MA, 02215, USA*
[2]*Electrical and computer Engineering Department, Boston University 8 St Mary's street, Boston, MA, 02215, USA*
[3]*Photonics Center, Boston University, 8 St Mary's street, Boston, MA, 02215, USA*
swan@bu.edu

Monolayer MoS2 has emerged as an excellent 2D semiconducting model system because of its two inequivalent, direct-gap valleys that lead to exotic bound and excited states. Here we focus on one such bound state, the negatively charged trion. Since trions are charged particles and are produced in abundance upon photoexcitation makes them interesting candidates for both scientific and technological pursuits because it is possible to control trion transport and density. Unlike excitons, trions can radiatively decay with non-zero momentum by kicking out an electron, resulting in an asymmetric trion photoluminescence (PL) peak with a long low-energy tail [1]. As a consequence, the PL peak position does not correspond to the zero momentum trion energy. Hence, the zero momentum trion energy, E_{0tr}, will be erroneously determined when using a symmetric, Lorentzian peak, which will result in over-estimating the trion binding energy.

Here we show that including the trion's long tail in our analysis we are able to accurately separate the exciton from the trion contributions to the PL spectra. According to theory, the asymmetric energy tail has both a size-dependent and a temperature-dependent contribution. Analysis of the temperature-dependent data reveals the effective trion size, consistent with literature, and the temperature dependence of the band gap and spin-orbit splitting of the valence band. Our model can be used to analyze trions in other systems such as MoSe2 and WSe2 and applied to heterostructures of TMDCs where only the interlayer excitons have been investigated. For interlayer trions, measuring the hole to electron mass ratio via the tail length as presented here would provide significant insight into which material donates the hole and which donates the electrons.

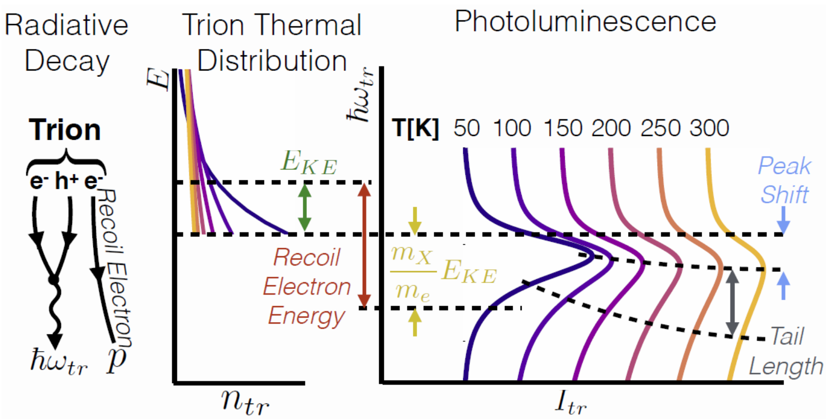

Figure 1. a) The radiative decay of trions allow for optical decay of particles with non-zero momentum. b) The momentum distribution of the trion depends on *T*. c) The recoil electron produces a temperature dependent asymmetric peak shape with a low energy tail.

Raman characterization of graphene has a long and illustrious history. The relative ease, speed, local information and non-destructive measurements makes Raman a valuable characterization tool to determine *e.g.*, strain, charge, layer thickness, defect concentration *etc*. Recent work by Lee *et al.* [2], showed that using statistically significant number of measurements, one can determine a samples local charge and strain state under certain conditions by using the relation between the 2D and G band positions. Here we focus on pristine graphene sandwiched in hBN and show that the Raman 2D peak split can be used as a good measure of very low charge density [3]. We revisit the origin of the asymmetry in the 2D peak that is observed at low doping [4,5] and screening effects on Fermi velocity and the TO phonon dispersion.

[1] Jason Christopher, Bennett Goldberg and Anna Swan, *arXiv*:1605.09741, 2016 - arxiv.org, (2016)
[2] JE Lee, G Ahn, J Shim, YS Lee, S Ryu - *Nature communications*, **3**, 1024 (2012)
[3] Xuanye Wang, Anna K Swan, In preparation. (2016).
[4] S Berciaud, X Li, H Htoon, LE. Brus, SK. Doorn, and TF. Heinz- *Nano Lett.*, **13** 3517–3523, (2013)
[5] Rohit Narula and Stephanie Reich, *Phys. Rev. B*, **90**, 085407, (2014)