Excitonic States in MoS_2

Farhang Fallah

IPM, School of Physics

Contents

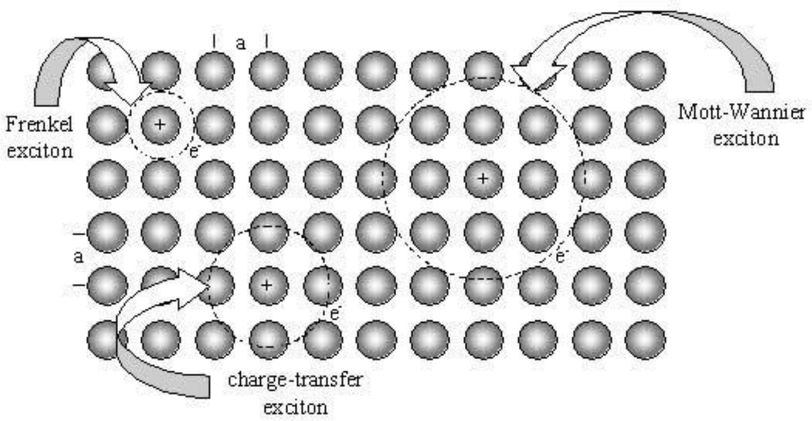
Excitons

- Bound states of electron and holes

- Two types:

- Frenkel

- Wannier-Mott



Frenkel Exciton

- Appears in materials with low dielectric constants (alkali halide crystals, organic molecular crystals, etc.)
- Low screening
- Binding Energy ~ 0.1 - 1 eV
- Bohr Radius ~ a few lattice constant

Wannier Exciton

- Appears in semiconductors
- High screening
- Binding Energy ~ 0.01 eV
- Bohr Radius ~ 10 – 100 × lattice constant

Excitons in Bulk Semiconductors

- Usually Wannier-type except in organic semiconductors

- Important in direct-band semiconductors e.g. III-V.

- Not much important in room temperature due to low binding energy (4 meV for GaAs)

Excitons in Lower Dimensions

- Considerably higher binding energy (~20 meV for typical quantum wells)

- Important optical effects in room temperature

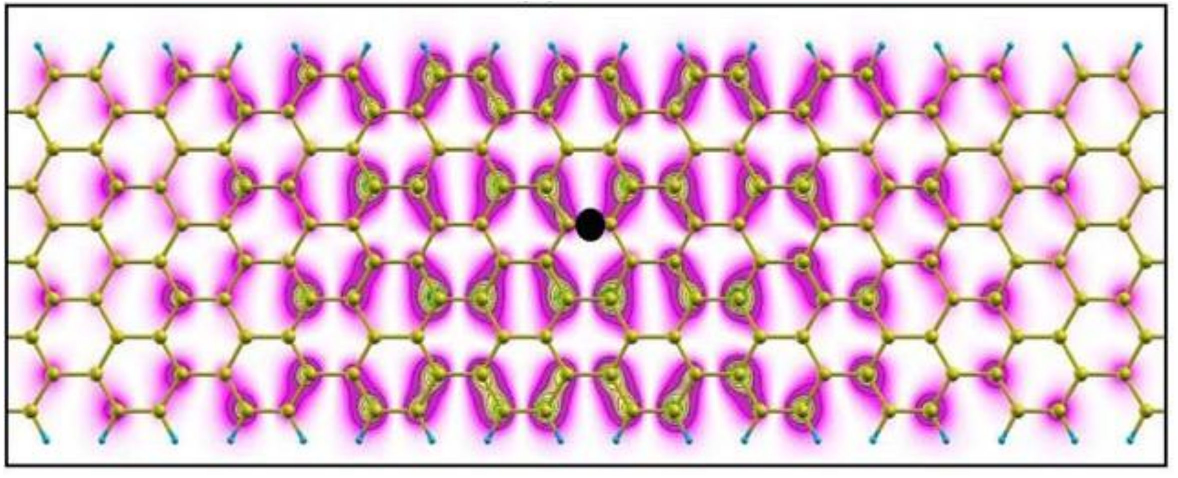
Excitons in Graphene

- Free-standing graphene → No gap → No Exciton
- We have to make an energy gap
- Size Effect → Graphene Nanoribbons
- Substrates (SiC, h-BN, etc.)

Excitons in Graphene

- Excitonic Effects in the Optical Spectra of Graphene Nanoribbons, L. Yang *et. Al.,* Nano Lett. **7**, 3112 (2007)

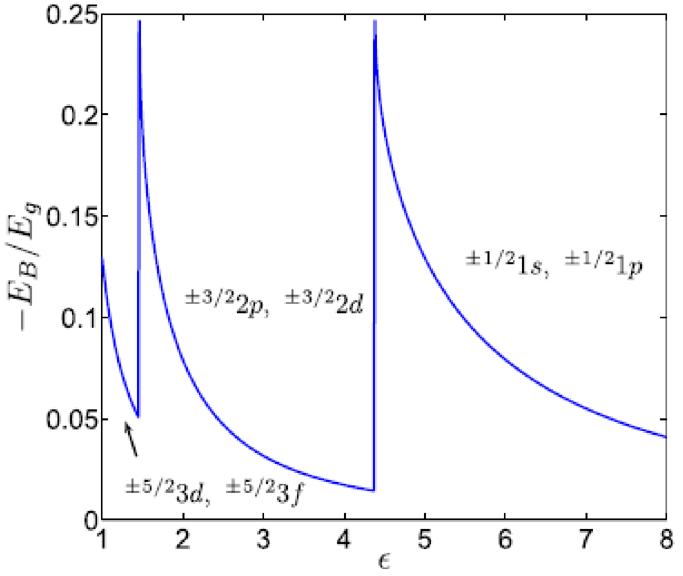
- High exciton binding energy (~ 1 eV for AGNR with w ~ 1.2 nm)

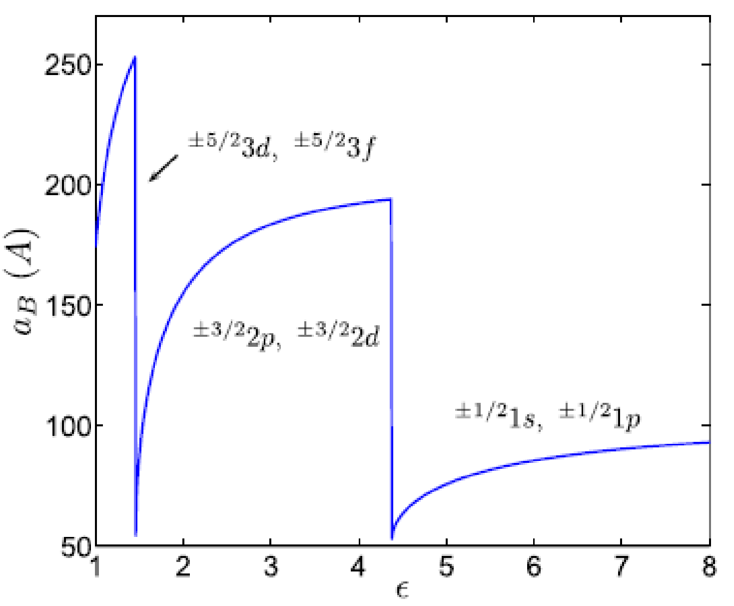


Excitons in Graphene

- Energy levels of exciton in a gapped graphene sheet, F. Fallah, M. Esmaeilzadeh, J. Appl. Phys. **114**, 073702 (2013).

$$E_{n,m} = \frac{\Delta}{2}\left\{1 + \frac{\alpha^2}{\left[n - |m| - \frac{1}{2} + (m^2 - \alpha^2)^{1/2}\right]^2}\right\}^{-1/2}$$

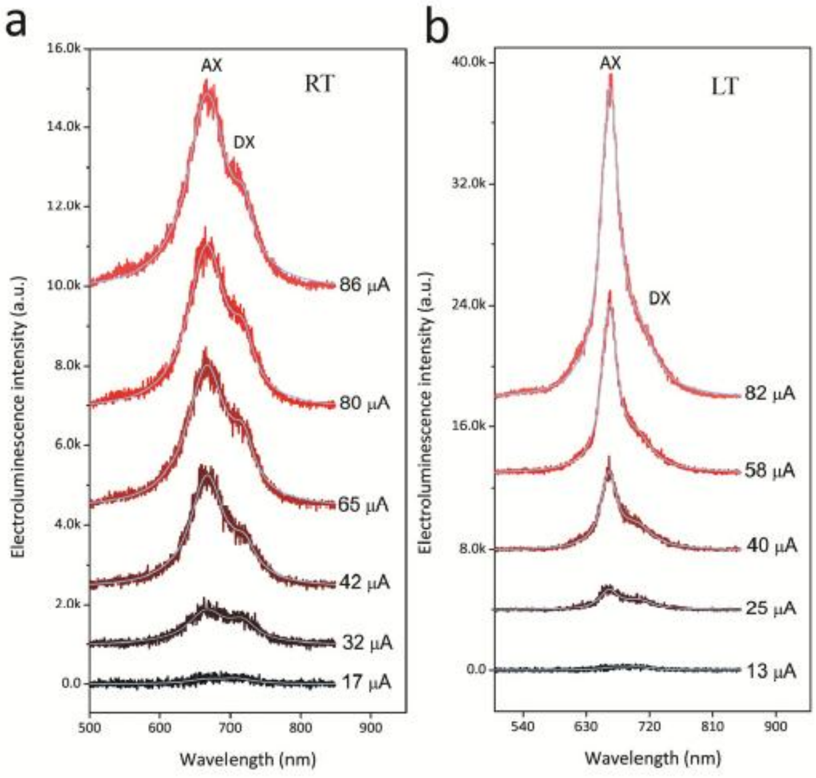




Excitons in MoS_2

- Exciton-related electroluminescence from monolayer MoS_2, Y. Ye, *et. al.,* arXiv:1305.4235 (2013).

- ~20 meV



Excitons in MoS_2

- Excitonic Collapse in Semiconducting Transition Metal Dichalcogenides, A. S. Rodin and A. H. Castro Neto, arXiv: 1305.4278 (2013)

- Exciton states collapse into the continuum states in the strong coupling regime

$$H = at(\tau k_x \sigma_x + k_y \sigma_y) + \frac{\Delta}{2}\sigma_z - \lambda\tau\frac{\sigma_z - 1}{2}s_z$$

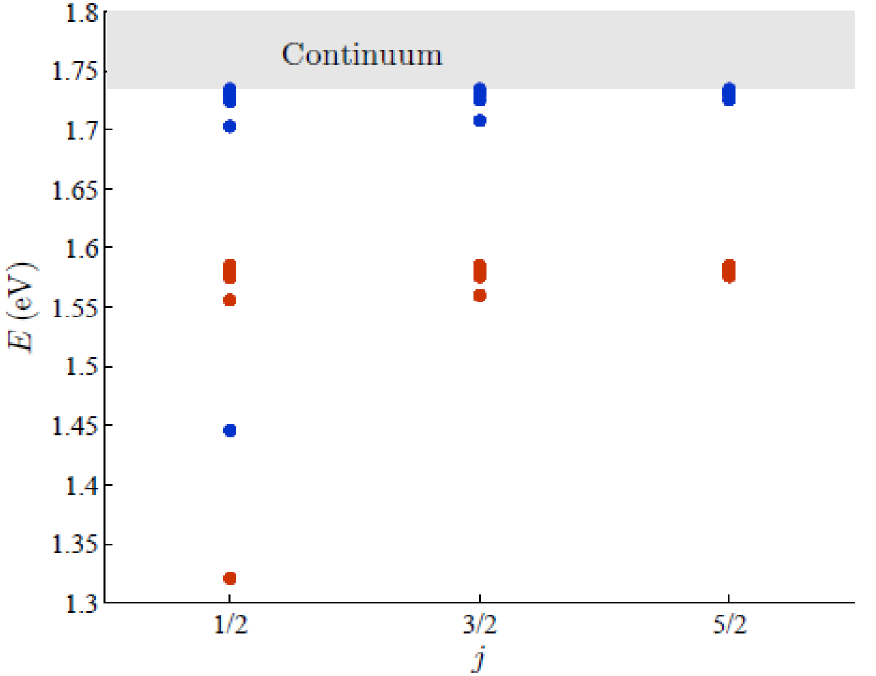
$$H_E = \begin{pmatrix} m_l & 2qe^{-i\theta} \\ 2qe^{i\theta} & -m_l \end{pmatrix} - \frac{\hbar v \alpha}{r}$$

Excitons in MoS_2

$$\mathcal{E}_{jn} = m_l \frac{n + \sqrt{j^2 - \bar{\alpha}^2}}{\sqrt{\bar{\alpha}^2 + \left[n + \sqrt{j^2 - \bar{\alpha}^2}\right]^2}} \qquad m_\pm = (\Delta \mp \lambda\tau)/(2\tau)$$

- SiC substrate (with dielectric constant of 5.5)

$$\bar{\alpha} \approx 0.42$$



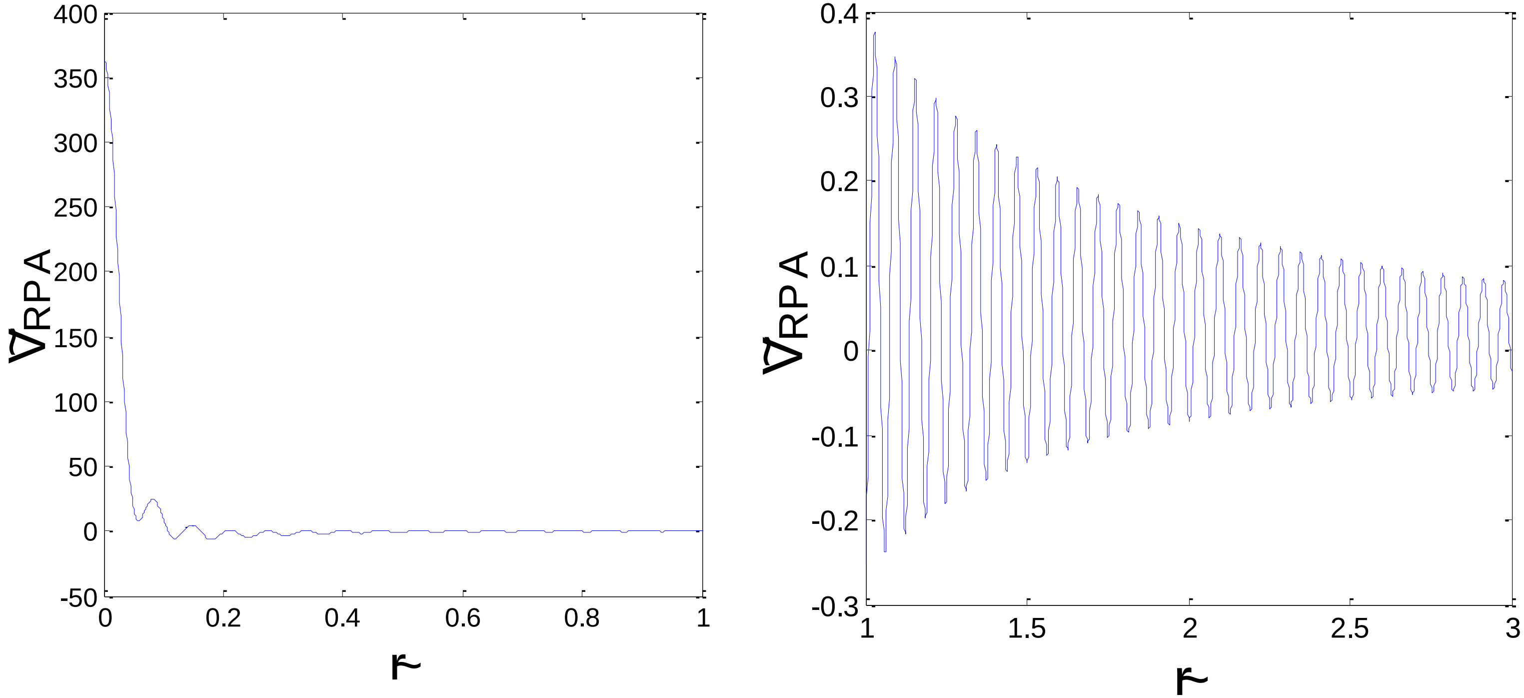
Excitons in MoS_2

- Effective lattice Hamiltonian for monolayer MoS2: Tailoring electronic structure with perpendicular electric and magnetic fields, H. Rostami, *et. Al.,* Phys. Rev. B **88**, 085440 (2013)

$$H_{\tau s} = \frac{\Delta}{2}\sigma_z + \lambda\tau s\frac{1-\sigma_z}{2} + t_0 a_0 \mathbf{q}\cdot\boldsymbol{\sigma}_\tau + \frac{\hbar^2|\mathbf{q}|^2}{4m_0}(\alpha+\beta\sigma_z) + t_1 a_0^2 \mathbf{q}\cdot\boldsymbol{\sigma}_\tau^* \sigma_x \mathbf{q}\cdot\boldsymbol{\sigma}_\tau^*$$

Excitons in MoS_2

- F. Fallah, R. Asgari (to be submitted)
- Effect of screening and non-zero β on excitonic states



Excitons in MoS_2

- non-zero β
- Different screening
- Collapsing Effect Disappears!

Thank You