Theory of Neutral Biexciton Clusters in Monolayer Transition Metal Dichalcogenides

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In latest years, there have been a promptly increasing number of experimental and theoretical publications focusing on transition metal dichalcogenides (TMD) materials. For example WS_2, WSe_2, MoS_2, $MoSe_2$ have been considered as potential materials “beyond grapheme”, allowing to use as a two dimentional (2D) semiconductors. The week dielectric screening and reduced dimensionality permitting the formation of excitons X (e^-e^+) (bound electron hole pairs) with binding energy few hundred mev. This behavior is not observed within three dimensional bulk medium and is unusual property of the TMD materials. Negative Trions X^- (eee^+) and biexcitons X_2 ($e\,ee^+\,e^+$), have also been observed.
The light emission measurements of trions and biexcitons introduced inconsistency between theory and experiment. This significant disagreement between the experimental results and the theoretical calculations is known as the "biexciton puzzle"[6].

Table 1. The experimental and theoretical biexciton binding energies (mev)

		WS_2	WSe_2	MoS_2	$MoSe_2$
Experiment	X_2	65[1]	52[2]	70[2]	-
Theory	X_2	24[3]	20[3]	22[3]	18[3]

We suggest a new theoretical analysis of the four-body 2D X2 (eee^+e^+) in the framework of the method of hyperspherical harmonics for solving four body Schrödinger equation [4]. We assume that electrons and holes are interacted via Keldysh potential [5]. This is the first time The convergences of binding energy calculations for the ground state of the trion as a function of the grand angular momentum are studied. For the biexcitons binding energy in MoS_2 we obtain 55.4 mev. This value is remarkably close to the experimental value. A comparison with results of other calculations is presented. We also study solutions of a hyperradial equation in a minimal approximation for the ground angular momentum to examine two regimes: a long range and a short range cases when the inter particle distance is much greater and much less than the screening length. For these cases, we find analytical expressions for the energy and wave function for biexciton states.

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This research is supported by Research PSC- CUNYGrant: award # PSC-CUNY Award # 69536-00 47