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Excitonic effects in 2D semiconductors: Path Integral Monte Carlo approach KIRILL VELIZHANIN, AVADH SAXENA, Los Alamos National Laboratory — One of the most striking features of novel 2D semiconductors (e.g., transition metal dichalcogenide monolayers or phosphorene) is a strong Coulomb interaction between charge carriers resulting in large excitonic effects. In particular, this leads to the formation of multi-carrier bound states (e.g., excitons, trions and biexcitons), which could remain stable at near-room temperatures and contribute significantly to optical properties of such materials. In my talk, I will report on our recent progress in using the Path Integral Monte Carlo methodology to numerically study properties of multi-carrier bound states in 2D semiconductors. Incorporating the effect of the dielectric confinement (via Keldysh potential), we have investigated and tabulated the dependence of single exciton, trion and biexciton binding energies on the strength of dielectric screening, including the limiting cases of very strong and very weak screening. The implications of the obtained results and the possible limitations of the used model will be discussed. The results of this work are potentially useful in the analysis of experimental data and benchmarking of theoretical and computational models.

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