Abstract

Two-dimensional transition metal dichalcogenides continue to evince enduring interest for decades now. A combination of low dimensionality, correlated electrons and inherent geometric frustration generates a complex, ill-understood phase diagram exhibiting unconventional charge-density-wave and superconductivity as a function of composition or pressure. Recent experimental work contradicts the long-held view of the charge density wave order arising from a nested band structure and van Hove singularity, at least in a subset of dichalcogenides family. An intrinsically strong coupling view, involving a charge density wave state arising as a Bose condensation of preformed excitons then emerges as an attractive, albeit scantily investigated, alternative. In this thesis, using an LCAO fit to the local density approximation combined with extended multi-orbital dynamical mean field theory, we show that the preformed excitonic liquid scenario shows excellent semi-quantitative agreement with a wide variety of extant normal state data in the transition metal dichalcogenides. Further, a genaralised Hartree-Fock mean field treatment of the effective Hamiltonian gives residual two particle interactions resulting in a charge density wave state, arising directly from two-particle instabilities of bad metallic normal state. Excellent quantitative explication of a wide range of spectral and transport responses in both, normal and CDW phases thus suggests Preformed Excitonic Liquid scenario as a novel theory for transition metal dichalcogenides.

In an annexure we also discuss our work on quantum criticality in a model as a separate study on a typical correlated model.

Keywords: Charge Density Wave, Superconductivity, Transition Metal Dichalcogenides, Dynamical Mean Field Theory.