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(G) (POS-64) Distortions of Transition Metal Dichalcogenides: Quantum Loops on the Triangular Lattice

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Transition Metal Dichalcogenides (TMDs) are layered semiconducting materials of the form MX_2, where M represents a transition metal atom and X represents a chalcogen. In the 1T structural phase, the chalcogens provide an octahedral environment for each metal atom. We propose a quantum loop model to explain the nature of bonding in these materials. We focus on metal atoms from group VI of the periodic table (e.g., MoS_2, $MoSe_2$, WS_2, WSe_2) which have two valence electrons in their d orbitals. These electrons reside in t_{2g} orbitals that point towards the six nearest neighbors on the underlying triangular lattice. We argue that these form covalent bonds that connect together to form loops. Loops can be formed in a large number of ways, leading to a resonating valence bond picture. We numerically enumerate all allowed loop configurations for small sizes of systems. We then construct a minimal effective Hamiltonian with local 'potential energy' and 'kinetic energy'terms. The kinetic energy term reflects processes where neighboring loops are cut and merged to form new loops, or a single loop changes shape. The potential energy term is due to the repulsion of proximate bonds. We construct a phase diagram, finding two prominent stripe-like phases. One of these closely resembles the 1T' structure, which is a well-known stripe-like distortion of the 1T phase. We discuss further tests of these ideas, e.g., in impurity-induced textures.

Keyword-1

TMDs

Keyword-2

Quantum loop model

Keyword-3

Author: Mr KNOWLES, Ashland (Brock University)

Co-authors: Dr BASKARAN, Ganapathy (Indian Institute of Technology, Madras; Perimeter Institute for Theoretical Physics, Waterloo); Dr RAMACHANDRAN, Ganesh (Brock University)

Presenter: Mr KNOWLES, Ashland (Brock University)

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