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Quantum loops in the 1T-transition metal dichalcogenides

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Dimer models and loop models have long been studied as prototypes for quantum ordering with local constraints. Robust physical realizations are not known, especially in solid state materials. We propose that a quantum loop model is indeed realized in MX_2, where M=Mo, W and X=S, Se or Te. In the single-layer 1T structure, each metal atom is in an octahedral chalcogen cage with two electrons in d orbitals. The geometry of the t_{2g} wavefunctions leads to highly directional overlaps between neighbouring metal atoms. Each metal atom participates in two covalent bonds, oriented towards two of the six nearest neighbours. These bonds connect to form loops on the underlying triangular lattice. We build a minimal model including local resonance processes and potential energy. We map out a phase diagram using exact diagonalization on small clusters. We find a phase that closely resembles the 1T' deformation seen in these materials. We discuss further experimental tests and consequences for other transition metal dichalcogenides.

Keyword-1

TMDs

Keyword-2

quantum spin liquids

Keyword-3

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