The Geometry of CDWs in Dichalcogenides

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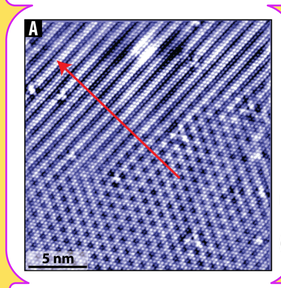
CDWs

STM image of $NbSe_2$



A. Soumyanarayanan et al. PNAS 110, 1623-1627 (2013)

'1Q' CDW, Stripe Order

Typically in crystalline materials the electron probability density has the symmetry of the ion lattice.

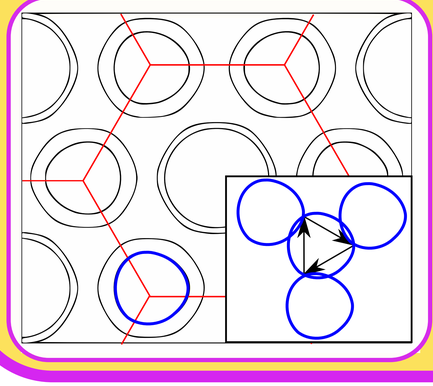
Under some conditions the symmetry of the electron field spontaneously breaks. The result is a charge density wave (CDW).

'3Q' CDW, Triangular Order
(3 x 1Q at π/3)

The CDW can take on different orientations and shapes, which can coexist by the production of domains.

The dichalcogenides $NbSe_2$and $TiSe_2$ demonstrate such a phenomenon.

Nesting in $NbSe_2$



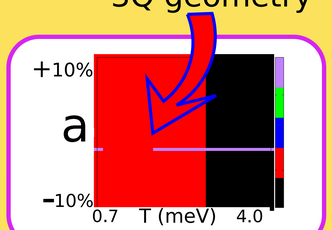
CDWs are often formed by Fermi surface nesting.

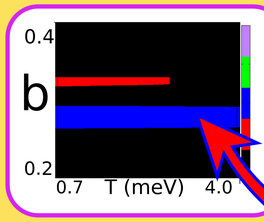
Part of the Fermi surface maps onto itself. Coupling the mapped states lowers the system's energy.

Evidence of nesting is unconvincing in $NbSe_2$.

Phase Diagrams

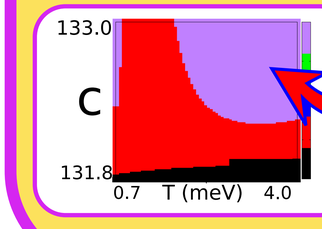
3Q geometry





$$g'(\mathbf{q}) = a\left(b - |\mathbf{q}|\right)^2 + c$$

3Q geometry, 1Q vector

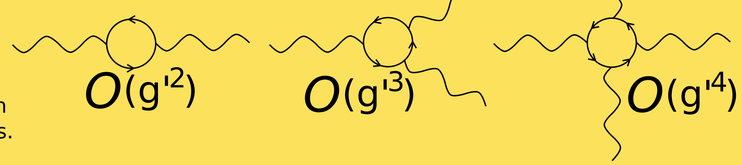


1Q geometry

Sensible forms, but quantitative disagreement with experiment - failing of weak coupling theory.

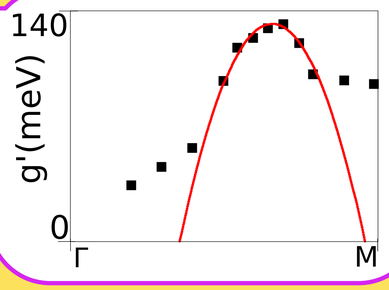
$NbSe_2$ Analysis: QFT

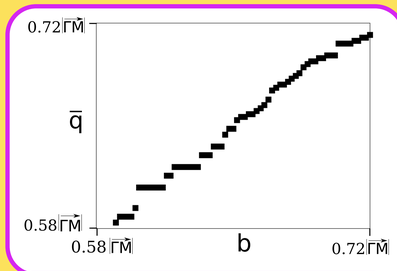
Free energy calculated using quantum field theory (QFT), including electron and phonon fields.



Expansion in Feynman diagrams to low order in electron-phonon coupling g' and with bare electron propagators: 'weak coupling'.

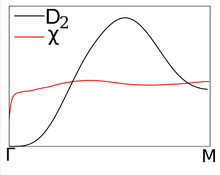
Form of g' estimated from renormalized phonon propagator plus experimental data: fit to quadratic.





Weak coupling predicts that value of momentum minimizing free energy (q) linear in g' peak location: phonon driven CDW transition.

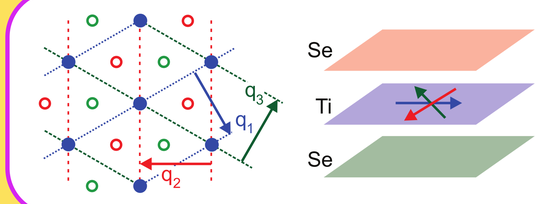
Weak coupling susceptibility χ flat around CDW ordering vector.



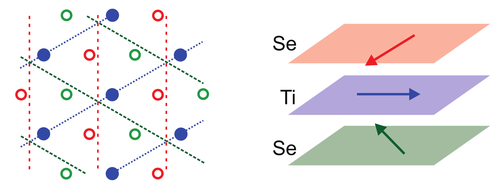
Strong coupling susceptibility D_2 peaked at observed CDW vector.

$TiSe_2$: Chiral Scalar Fields

Achiral 3Q CDW



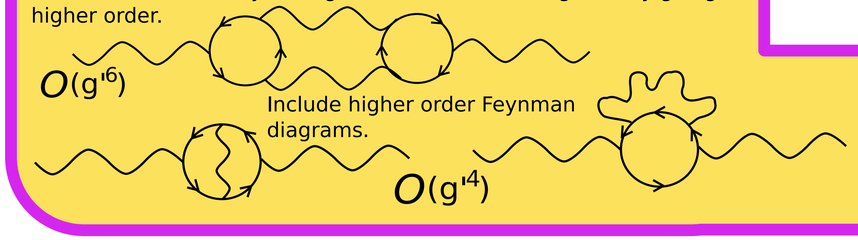
J. van Wezel, EPL 96, 67011 (2011)



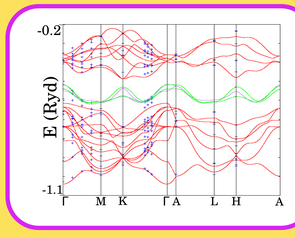
Chiral 3Q CDW

Stronger Coupling QFT

Weak coupling shows phonons drive the CDW transition. Increase their role in the theory through a full calculation of g' and by going to higher order.



Calculate electron-phonon coupling theoretically and check against experiment.



Finding g' requires a calculation of the full electron bandstructure: tight binding fit, Monte Carlo minimization to combination of ARPES and LDA.