Spin-Peierls Instability

Coupling of electronic and lattice degrees of freedom leads to interesting physics already in one dimension:

- Peierls instability of 1D metals towards lattice distortions
- Mott to Peierls insulator transition in the 1D Holstein-Hubbard model
- Spin-Peierls instability in spin chains with magnetoelastic coupling

Physical examples for the latter were found in quasi-1D organic materials (TTF/TCNQ) as well as in 1D organic metals (e.g., in quasi-1D organic materials (TTF/TCNQ) as well as in 1D organic metals (e.g., bilayer Cu2OCl2) [62].

Microscopic Models

Microscopic models comprise a Heisenberg spin-1/2 chain and a set of Einstein oscillators coupled by an interaction term:

\[ H = \sum_i [\vec{S}_i \cdot \vec{S}_{i+1} + \omega_i (\vec{b}_i \cdot \vec{b}_{i+1}) + H_{pp}], \]

with common choices for the coupling:

\[ H_{pp} = g_0 \sum_i [\vec{b}_i \cdot (\vec{S}_i \cdot \vec{S}_{i+1}) - \vec{S}_i \cdot \vec{S}_{i+1} + H_{pp}], \]

and, respectively:

\[ H_{pp} = g_0 \sum_i [\vec{b}_i \cdot (\vec{S}_i \cdot \vec{S}_{i+1}) - \vec{S}_i \cdot \vec{S}_{i+1}]. \]

All analytical and numerical approaches so far agree on the following scenarios:

- weak coupling: spin liquid, gaps
- strong coupling: lattice dimerization, massive spin excitations

The basic mechanism of the phase transition is well understood — effective spin interactions beyond nearest-neighbors lead to effective low-dimensional models, which are known to susceptible to dimension reduction beyond some critical frustration.

Example: In the (interacting) Heisenberg chain

\[ H = \sum_i [\vec{S}_i \cdot \vec{S}_{i+1} + \alpha \vec{S}_i \cdot \vec{S}_{i+1}], \]

dimensionality sets in at \( \alpha = 0.241467 \) [28].

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References