RPA studies of the Spin-Peierls Transition

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Motivation

- First inorganic spin-Peierls (SP) material $CuGeO_3$: Displacive SP transition at $T_{SP} = 14.1K$. No soft phonon found experimentally.
- Nature of the SP-transition: soft mode vs. central peak behaviour?
- Ultrasound signature at phase transition?

Minimal Model

$$H = H_{Ph} - \sum_i J(R_i - R_{i+1})(S_{i,x}S_{i+1,x} + S_{i,y}S_{i+1,y})$$

$$H_{Ph} = \sum_i \frac{p_i^2}{2m} + \frac{K}{2}(u_i - u_{i+1})^2$$

1D XY-Model with position-dependent exchange integral

$$J(R_i - R_{i+1}) = J(R_i^0 + u_i - R_{i+1}^0 - u_{i+1}) \approx J + g\cdot(u_i - u_{i+1})$$

including the coupling to phonons (in linear approximation)

RPA-Treatment

☐ Uniform Phase

- Hamiltonian (Jordan-Wigner and Fourier transformed):

$$\begin{aligned}\tilde{H}^U &= \tilde{H}_m^U + \tilde{H}_{Ph}^U + \tilde{H}_{int}^U \\ &= \sum_q \tilde{\omega}_q a_q^\dagger a_q + \sum_k \tilde{\varepsilon}_k^U d_k^\dagger d_k \\ &\quad + \sum_{k,q} g_{k,q}^U (a_q + a_{-q}^\dagger) d_k^\dagger d_{k-q}\end{aligned}$$

$$g_{k,q}^U = -i\left(\frac{\tilde{\lambda}\tilde{\omega}_\pi^2 \pi}{\tilde{\omega}_q N}\right)^{\frac{1}{2}} [\sin(k-q) - \sin(k)]$$

$$\tilde{H} = \frac{H}{J} \quad \tilde{\omega} = \frac{\omega}{J} \quad \tilde{\varepsilon}_k^U = -\cos(k)$$

$$\tilde{\lambda} = \frac{g^2}{8\pi K J} \quad \tilde{\beta} = \frac{J}{T} \quad \tilde{\omega}_n = \frac{2n\pi}{\tilde{\beta}}$$

- Matsubara Green's function for a phonon with $q = \pi$:

$$\tilde{D}(\pi, i\tilde{\omega}_n) = \frac{2\tilde{\omega}_\pi}{(i\tilde{\omega}_n)^2 - \tilde{\omega}_\pi^2 - 2\tilde{\omega}_\pi \tilde{P}(\pi, i\tilde{\omega}_n)}$$

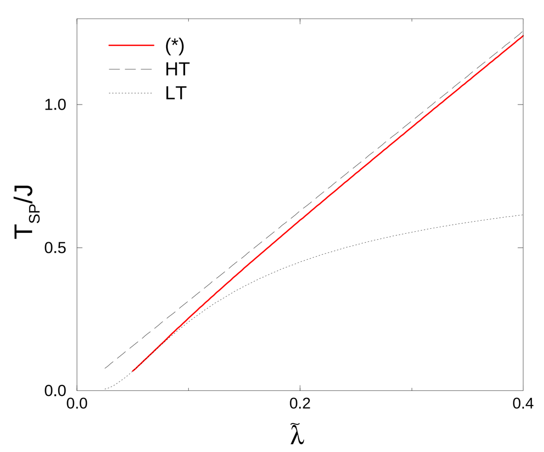
$$\tilde{P}(\pi, i\tilde{\omega}_n) = -4\tilde{\lambda}\tilde{\omega}_\pi \int_0^\pi dk \sin^2(k) \frac{\tanh\left(\frac{\tilde{\beta}}{2}\cos(k)\right)}{i\tilde{\omega}_n + 2\cos(k)}$$

- Analytic continuation of retarded Green's function to the lower complex half-plane ⇒ two branches (one accesible directly, one by extrapolation)

- SP-transition is always connected to a pole at $\tilde{\omega} = 0$

$$\Rightarrow \quad 1 = 4\tilde{\lambda}\int_0^\pi dk \sin^2(k)\frac{\tanh\left(\frac{\tilde{\beta}_{SP}}{2}\cos(k)\right)}{\cos(k)} \quad (*)$$

Dependence of T_{SP} on $\tilde{\lambda}$



Solution of (∗) compared to the high-temperature ($\tilde{\lambda} \gg 1$, HT) and low-temperature ($\tilde{\lambda} \ll 1$, LT) results.

☐ Dimerized Phase

- $T = T_{SP}$: Instability of lattice against dimerization. Transformation: $u_l \to u_l - \frac{1}{2}(-1)^l\delta$ ⇝ lattice period doubles ⇒ $q \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$; one acoustical ($\nu = 0$) and one optical ($\nu = 1$) phonon branch.
- Hamiltonian (after several transformations cf. Ref. [1]):

$$\begin{aligned}\tilde{H}^D &= \tilde{H}_m^D + \tilde{H}_{Ph}^D + \tilde{H}_{elast}^D + \tilde{H}_{II}^D + \tilde{H}_{int}^D \\ &= {\sum_k}' \tilde{\varepsilon}_k^D(\gamma_k^\dagger\gamma_k - \beta_k^\dagger\beta_k) + {\sum_{q,\nu}}' \tilde{\omega}_{q,\nu} a_{q,\nu}^\dagger a_{q,\nu} \\ &\quad + \frac{N\tilde{\delta}^2}{16\pi} - \frac{\tilde{\delta}\sqrt{N}}{4\sqrt{\pi}}(a_{0,1} + a_{0,1}^\dagger) \\ &\quad + {\sum_{k,q,\nu}}' g_{k,q,\nu}^D (a_{q,\nu} + a_{-q,\nu}^\dagger) \\ &\qquad \left[\left(\beta_k^\dagger\beta_{k-q} - \gamma_k^\dagger\gamma_{k-q}\right)\cdot T_{k,q,\nu} \right. \\ &\qquad \left. - \left(\beta_k^\dagger\gamma_{k-q} - \gamma_k^\dagger\beta_{k-q}\right)\cdot T_{k,q,\nu+1}\right]\end{aligned}$$

$$g_{k,q,\nu}^D = -i\left(\frac{\pi\tilde{\omega}_\pi^2\tilde{\lambda}}{4N\tilde{\omega}_{q,\nu}}\right)^{\frac{1}{2}}[\sin(k) - (-1)^\nu \sin(k-q)]$$

$$T_{k,q,\nu} = \left(e^{i\Theta_{k-q}} + \alpha_{k-q}(-1)^\nu e^{-i\Theta_k}\right) \qquad \tilde{\delta} = \sqrt{\frac{8\pi K}{J}}\delta$$

$$\tilde{\varepsilon}_k^D = \sqrt{\cos^2(k) + \tilde{\lambda}\tilde{\delta}^2\sin^2(k)} = \tilde{\varepsilon}_k^\gamma = -\tilde{\varepsilon}_k^\beta$$

$$\Theta_k = \arctan\left(\sqrt{\tilde{\lambda}}\tilde{\delta}\tan(k)\right) \quad \alpha_{k-q} = \mathrm{sgn}\left(\frac{\pi}{2} - |k-q|\right)$$

- Phonon propagator

$$\tilde{D}(q,\nu,i\tilde{\omega}_n) = \tilde{D}_0(q,\nu,i\tilde{\omega}_n) \times \frac{1 - \sum_{\mu\neq\nu}\tilde{D}_0(q,\mu,i\tilde{\omega}_n)\tilde{P}(q,\mu,i\tilde{\omega}_n)}{1 - \sum_\mu \tilde{D}_0(q,\mu,i\tilde{\omega}_n)\tilde{P}(q,\mu,i\tilde{\omega}_n)}$$

$$\begin{aligned}\tilde{P}(q,\nu,i\tilde{\omega}_n) &= \frac{\tilde{\lambda}\tilde{\omega}_\pi^2}{4\tilde{\omega}_{q,\nu}}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} dk(\sin(k) - (-1)^\nu\sin(k+q))^2 \\ &\quad \times\left\{\Lambda(k,q,\nu)(K^{\beta,\beta}(k,q,i\tilde{\omega}_n) + K^{\gamma,\gamma}(k,q,i\tilde{\omega}_n)\right. \\ &\quad \left. + \Lambda(k,q,\nu+1)(K^{\beta,\gamma}(k,q,i\tilde{\omega}_n) + K^{\gamma,\beta}(k,q,i\tilde{\omega}_n)\right\}\end{aligned}$$

$$\Lambda(k,q,\nu) = (1 + \alpha_{k+q}(-1)^\nu\cos(\Theta_k + \Theta_{k+q}))$$

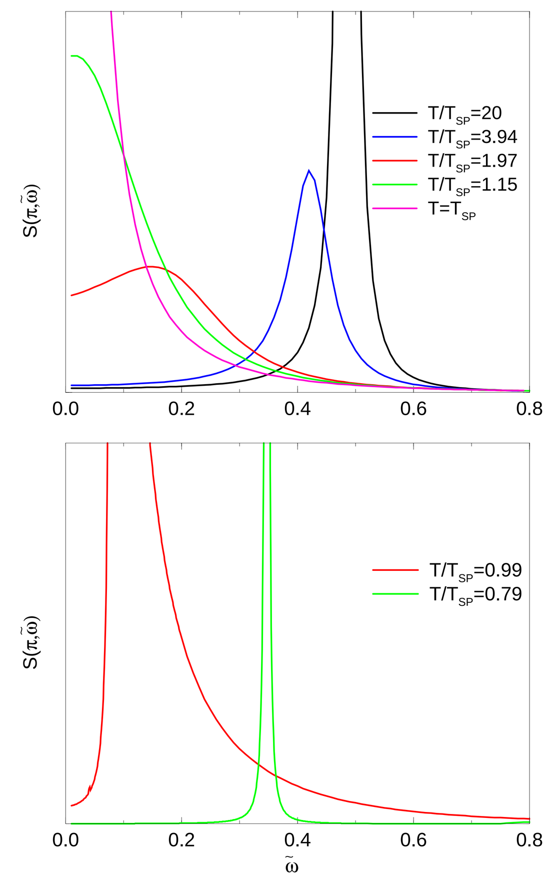
$$K^{x,y}(k,q,i\tilde{\omega}_n) = \frac{n_F^x(k+q) - n_F^y(k)}{i\tilde{\omega}_n + \tilde{\varepsilon}_{k+q}^x - \tilde{\varepsilon}_k^y}$$

☐ Results

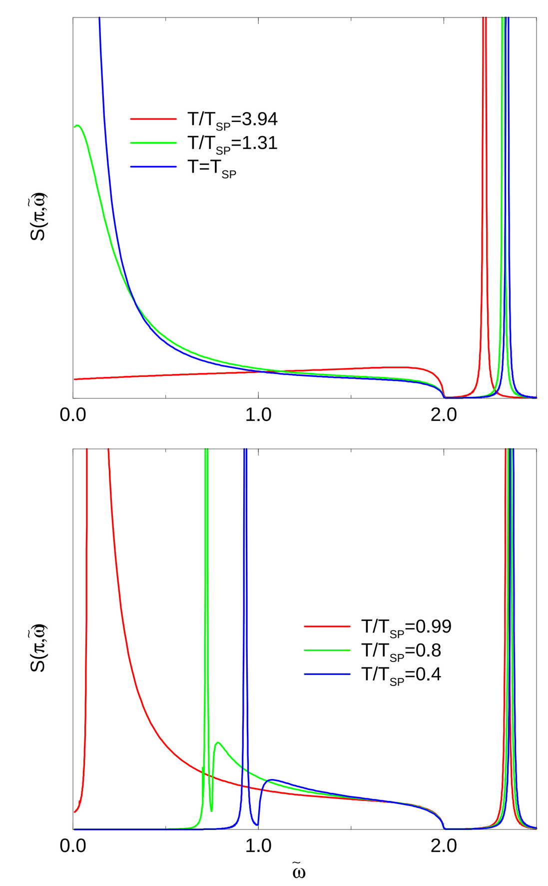
- Dynamical phonon structure factor:

$$S(q,\tilde{\omega}) = -\frac{1}{\pi}\lim_{\delta\to 0}\frac{\sum_\nu \mathrm{Im}\tilde{D}^{ret}(q,\nu,\tilde{\omega}+i\delta)}{1 - e^{-\tilde{\beta}\tilde{\omega}}}$$

Soft mode regime ($\tilde{\omega}_\pi = 0.5$, $\tilde{\lambda} = 0.1$)

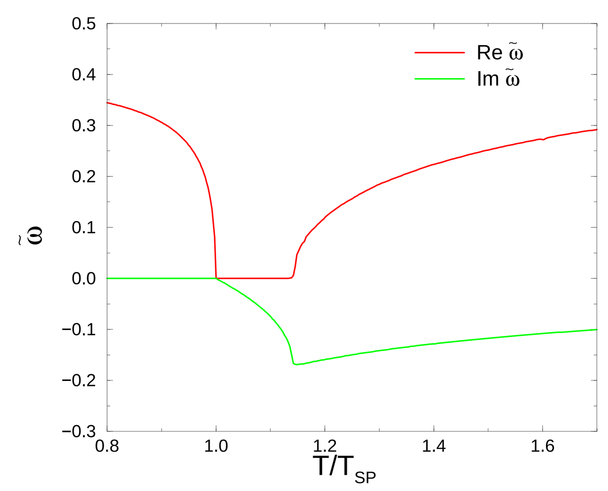


Central peak regime ($\tilde{\omega}_\pi = 2.1$, $\tilde{\lambda} = 0.1$)

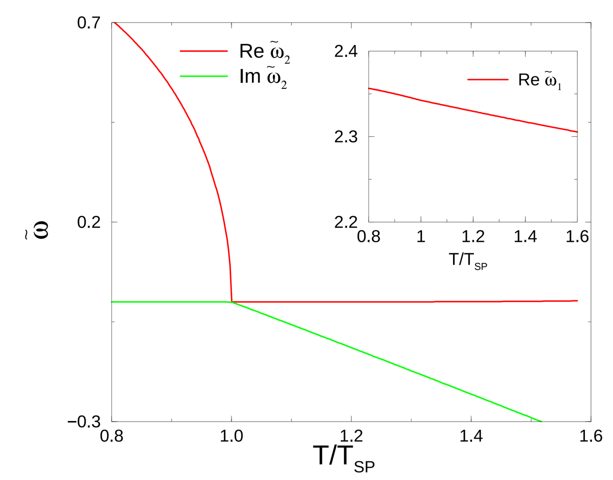


- Poles of the retarded Green's function yield the renormalized phonon frequencies.

Soft mode regime ($\tilde{\omega}_\pi = 0.5$, $\tilde{\lambda} = 0.1$)



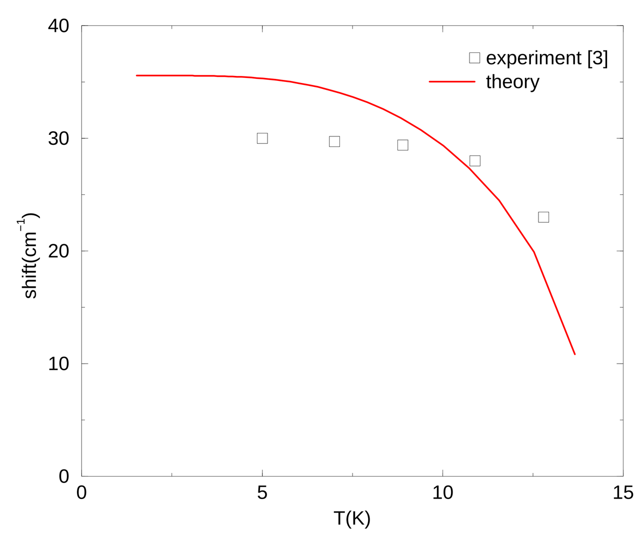
Central peak regime ($\tilde{\omega}_\pi = 2.1$, $\tilde{\lambda} = 0.1$)



☐ Application to $CuGeO_3$

- Values from [2]:
  - Transition temperature $T_{SP} = 14.1K$
  - Exchange integral $J = 150K$
  - Frequency of mode with strongest coupling $\Omega_\pi/2\pi = 6.53THz$
- Give the system parameters $\tilde{\omega}_\pi = 2.09$, $\tilde{\lambda} = 0.057$
- Spin gap: $2\Delta = 2\sqrt{\tilde{\lambda}}\tilde{\delta}\cdot J = 4.422meV$ compared to experiment [3] $2\Delta = 4.2meV$
- Exchange alternation $\delta_J = \sqrt{\tilde{\lambda}}\tilde{\delta} = 0.1645$
- Is the experimentally found $30cm^{-1}$-mode a relict of the central peak?

Central peak energy vs. temperature ($\tilde{\lambda} = 0.057$, $\tilde{\omega}_\pi = 2.09$) compared to $30cm^{-1}$-mode in $CuGeO_3$



Landau Approach

- Minimization of free energy

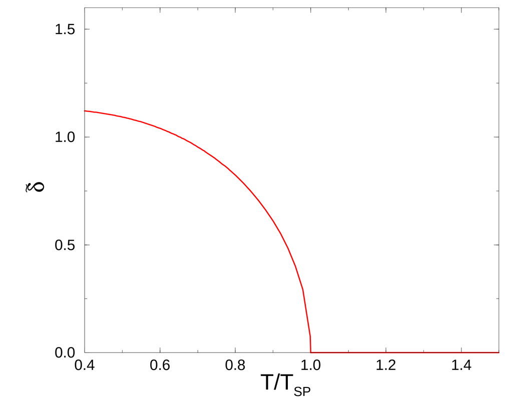
$$f = -\frac{1}{N\tilde{\beta}}\ln\langle\exp(-\tilde{\beta}(\tilde{H}_m^D + \tilde{H}_{elast}^D))\rangle$$

with respect to $\tilde{\delta}$ gives

$$1 = 8\tilde{\lambda}\int_0^{\frac{\pi}{2}} dk \frac{\tanh(\frac{\tilde{\beta}}{2}\tilde{\varepsilon}^D(k))}{\tilde{\varepsilon}^D(k)}\sin^2(k)$$

for the determination of the static dimerization $\tilde{\delta}$, where $\langle(a_{0,1} + a_{0,1}^\dagger)\rangle = 0$.
⇝ Interpretation of $\tilde{\delta}$ as **order parameter**

Order parameter vs. temperature ($\tilde{\lambda} = 0.1$)



- Coupling of external strain $\tilde{\epsilon}$ to the system ⇝ additional term $\tilde{H}_{elastII}^D$ in Hamiltonian and change of J

$$\tilde{H}_{elastII}^D = \frac{N\tilde{\epsilon}^2}{16\pi} \qquad J \to J + \frac{g}{\sqrt{2\pi mJ\tilde{\omega}_\pi}}\tilde{\epsilon}$$

- Expansion of free energy for small $\tilde{\delta}$ and $\tilde{\epsilon}$

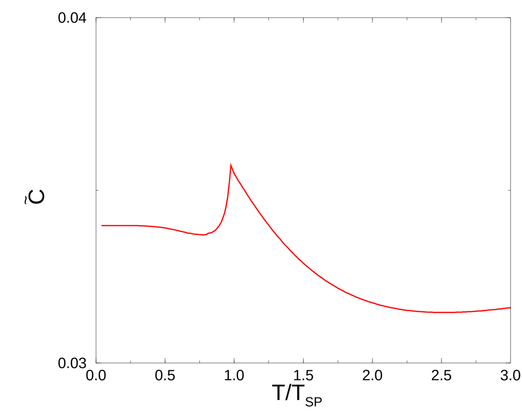
$$f = a_0 + a_2\tilde{\delta}^2 + a_4\tilde{\delta}^4 + b_0\tilde{\epsilon} + b_2\tilde{\epsilon}\tilde{\delta}^2$$

⇝ Strain couples to square of order parameter

- Elastic modulus

$$\tilde{C} = \frac{d^2}{d\tilde{\epsilon}^2}f(\tilde{\epsilon},\tilde{\beta},\tilde{\delta}(\tilde{\epsilon},\tilde{\beta}))$$

Elastic modulus vs. temperature ($\tilde{\lambda} = 0.1$)



Conclusions

- In dependence on $\tilde{\omega}_\pi$ RPA gives two distinct regimes, a soft-mode and a central peak regime.
- Appearance of a second excitation in the central peak regime with an energy of the same order of magnitude as the $30cm^{-1}$-mode.
- Experimentally found [4] strain-order parameter coupling can be derived from microscopic theory.

Outlook

- Derivation of ultrasound anomaly via Green's function formalism would be desirable.
- Going beyond RPA ⇝ method of Self Consistent Renormalization

References

[1] R. Lima, C. Tsallis, Phys. Rev. B 27, 6896 (1983)
[2] R. Werner, C. Gros, M. Braden, Phys. Rev. B 59, 14356 (1999)
[3] G. Els et al., Phys. Rev. Lett. 79, 5138 (1997)
[4] M. Saint-Paul et al., Solid State Commun. 93, 7 (1995)