A8

Interacting magnons and critical behavior of bosons

Part B: Theory of ultrasound in the vicinity of the dilute Bose gas critical point

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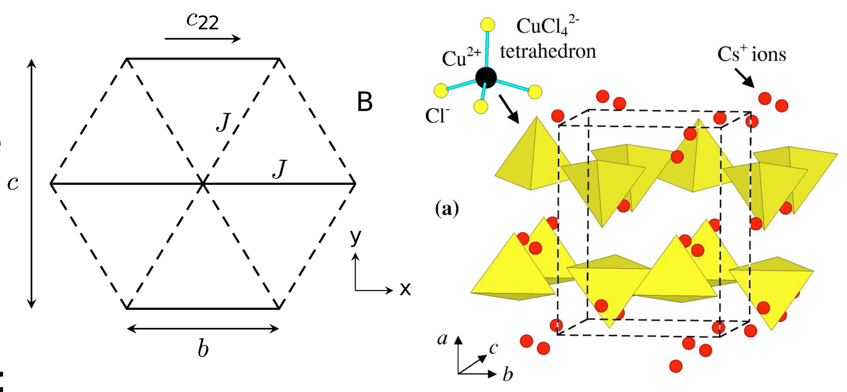
Cs_2CuCl_4

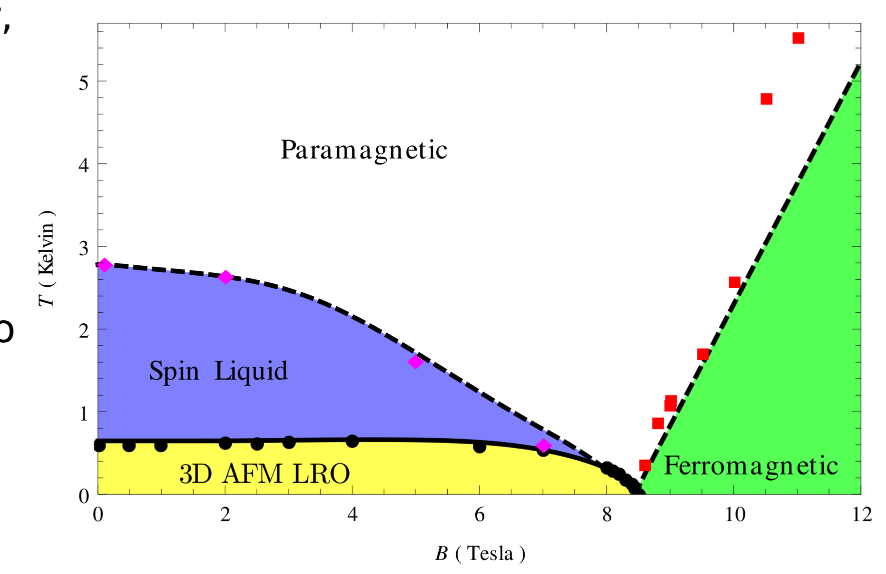
- motivation: ultrasound physics (c_{22}-mode) in the spin-liquid phase of Cs_2CuCl_4
- crystal structure: orthorhombic ($Pnma$)
- Cu^{2+}: carry spin 1/2 (orbital quenching) and form a triangular lattice in each plane
- effective 2D Hamiltonian with $B \parallel a$:
  $$\mathcal{H} = \frac{1}{2}\sum_{ij} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j - h\sum_i S_i^z \quad \text{with } h = g\mu_B B, \quad g = 2.2$$
- two nearest neighbor exchange couplings: $J = 4.34\text{K}$ and $J' = 1.49\text{K}$ ($k_B \equiv 1$) [Coldea *et al.*, PRL 2002] (from neutron scattering data in the ferromagnetic phase)



[Coldea *et al.*, PRB 2003]

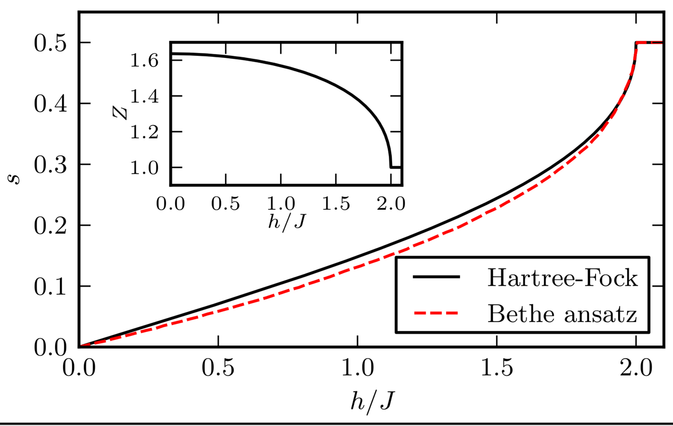
Phase diagram: spin-liquid phase

- spin-liquid phase: no long-range order, but strong short-range correlations
- inelastic neutron scattering: highly dispersive excitation continua, signature of spin-1/2 spinons [Coldea *et al.*, PRB 2003]
- quasi-one-dimensional behavior due to frustration and quantum fluctuations
- dilute Bose gas quantum critical point at $B_c = 8.5\,\text{T}$: BEC of magnons [Radu *et al.*, PRL 2005]



Heisenberg chain coupled to phonons

- spin-phonon Hamiltonian: $\mathcal{H} = \sum_n J_n [\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1} - 1/4] - h\sum_n S_n^z + \mathcal{H}_2^p$
- one-dimensional phonons: $\mathcal{H}_2^p = \sum_q \left[\frac{P_{-q}P_q}{2M} + \frac{M}{2}\omega_q^2 X_{-q}X_q\right], \quad \omega_q = c\frac{|q|}{b}$
- exchange-striction mechanism: $J_n \approx J + J^{(1)}(X_{n+1} - X_n) + \frac{J^{(2)}}{2}(X_{n+1} - X_n)^2$
- Jordan-Wigner transformation to spinless fermions:
  $$S_n^+ = c_n^\dagger(-1)^n e^{i\pi\sum_{j<n} c_j^\dagger c_j}, \quad S_n^- = (-1)^n e^{-i\pi\sum_{j<n} c_j^\dagger c_j} c_n, \quad S_n^z = c_n^\dagger c_n - 1/2$$
  $$\mathcal{H} = -\frac{1}{2}\sum_n J_n(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n + c_n^\dagger c_n + c_{n+1}^\dagger c_{n+1}) + \sum_n J_n c_n^\dagger c_n c_{n+1}^\dagger c_{n+1} - h\sum_n c_n^\dagger c_n + Nh/2 + \mathcal{H}$$
- self-consistent Hartree-Fock theory:
  $$c_n^\dagger c_n c_{n+1}^\dagger c_{n+1} \approx \rho(c_{n+1}^\dagger c_{n+1} + c_n^\dagger c_n) - \rho^2 - \tau(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + \tau^2$$
- self-consistency conditions: $\rho = \langle c_n^\dagger c_n\rangle$, $\tau = \langle c_n^\dagger c_{n+1}\rangle$
- fermion dispersion: $\xi_k = -ZJ\cos k + 2sJ - h$
- renormalization of the hopping: $Z = 1 + 2\tau$
- dimensionless magnetization: $s = \rho - 1/2$

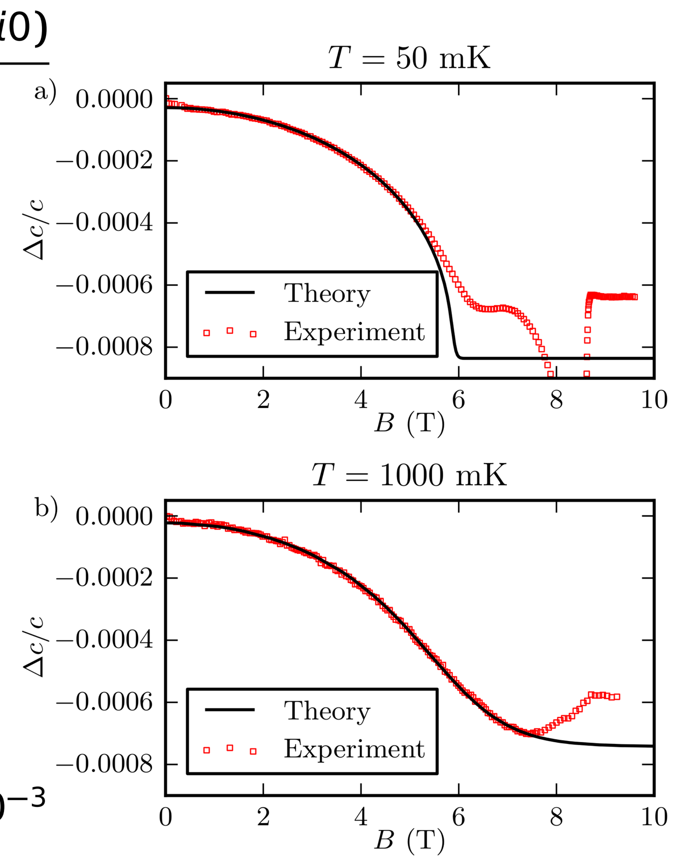


Spin-phonon coupling

- approximate spin-phonon Hamiltonian: $\mathcal{H} = F_0 + \sum_k \xi_k c_k^\dagger c_k + \mathcal{H}_2^p + \delta\mathcal{H}_2^p + \mathcal{H}_3^{sp} + \mathcal{H}_4^{sp}$
  $$F_0/N = h/2 + J(\tau^2 - \rho^2), \quad \delta\mathcal{H}_2^p = 2J^{(2)}(\tau^2 - \rho^2)\sum_q \sin^2(q/2)X_{-q}X_q$$
  $$\mathcal{H}_3^{sp} = \frac{1}{\sqrt{N}}\sum_{k'kq}\delta^*_{k',k+q}\Gamma_3(k,q)c_{k'}^\dagger c_k X_q$$
  $$\mathcal{H}_4^{sp} = \frac{1}{2N}\sum_{k'kq_1q_2}\delta^*_{k',k+q_1+q_2}\Gamma_4(k,q_1,q_2)c_{k'}^\dagger c_k X_{q_1}X_{q_2}$$
  $$\Gamma_3(k,q) \approx -iqJ^{(1)}[Z\cos k - 2s], \quad \Gamma_4(k,q_1,q_2) \approx q_1q_2J^{(2)}[Z\cos k - 2s]$$
- propagator of the phonon field X_q: $\langle X_{q,\omega}X_{-q,-\omega}\rangle = \frac{\beta N}{M}\frac{1}{\omega^2 + \omega_q^2 + \Pi(q,i\omega)}$
- phonon self-energy: $\Pi(q,i\omega) = \Pi_2(q) + \Pi_3(q,i\omega) + \Pi_4(q)$
  $$\Pi_2(q) = [J^{(2)}/M][\tau^2 - \rho^2]4\sin^2(q/2), \quad \Pi_4(q) = \frac{1}{MN}\sum_k f_k\Gamma_4(k,q,-q)$$
  $$\Pi_3(q,i\omega) = \frac{1}{MN}\sum_k \frac{f_k - f_{k+q}}{\xi_k - \xi_{k+q} + i\omega}|\Gamma_3(k,q)|^2, \quad f_k = \frac{1}{e^{\beta\xi_k} + 1}$$

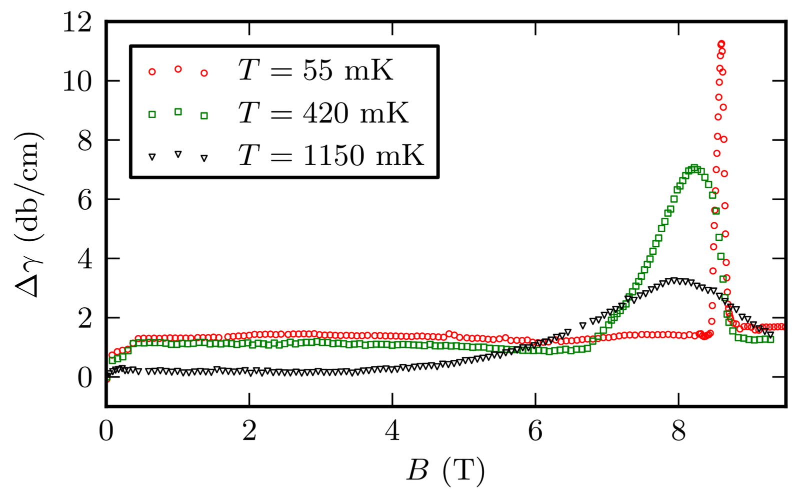
Sound velocity (c_{22}-mode)

- renormalized dispersion: $\tilde{\omega}_q = \omega_q + \frac{\mathrm{Re}\Pi(q,\omega_q + i0)}{2\omega_q}$
- renormalized sound velocity: $\tilde{c} = \lim_{q\to 0}\tilde{\omega}_q/q$
- shift of the sound velocity: $\Delta c = \tilde{c} - c$
  $$\Delta c/c = g_1c^{(1)} + g_2c^{(2)}$$
  $$c^{(1)} = \int_{-\pi}^{\pi}\frac{dk}{2\pi}Jf'(\xi_k)\frac{v_k}{v_k - c}[2s - Z\cos k]^2$$
  $$c^{(2)} = s^2 - Z^2/4$$
- dimensionless coupling constants:
  $$g_1 = [J^{(1)}b]^2/(2Mc^2J), \quad g_2 = J^{(2)}b^2/(2Mc^2)$$
- group velocity of the fermions: $v_k = ZJb\sin k$
- Cs_2CuCl_4: $c/(Jb) \approx 6.8 \Rightarrow c^{(2)} \gg c^{(1)}$ ($\hbar \equiv 1$)
- fit to experimental data: $g_1 \approx 0$, $g_2 \approx -1.1 \times 10^{-3}$

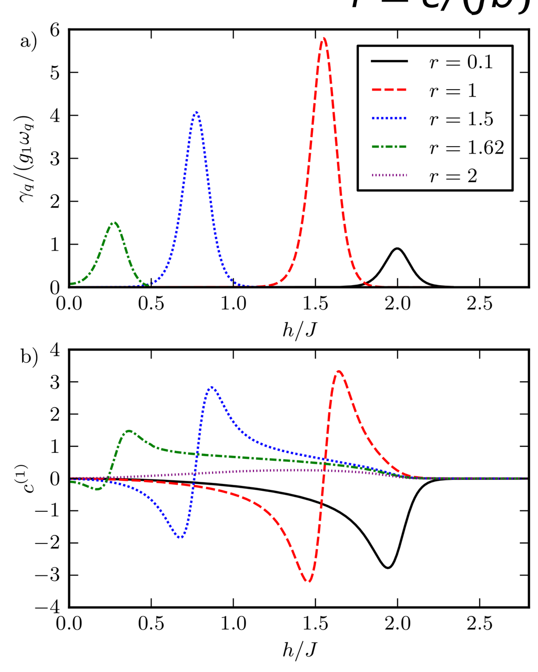


Ultrasound attenuation (c_{22}-mode)

- phonon damping:
  $$\gamma_q = -\frac{\mathrm{Im}\Pi(q,\omega_q + i0)}{2\omega_q} = \frac{\pi}{2M\omega_q}\int_{-\pi}^{\pi}\frac{dk}{2\pi}(f_k - f_{k+q})|\Gamma_3(k,q)|^2\delta(\xi_k - \xi_{k+q} + \omega_q)$$
- limit $q \to 0$: $\frac{\gamma_q}{\omega_q} \sim \frac{g_1cJ\Theta(v_*^2 - c^2)}{2v_*\sqrt{1 - c^2/v_*^2}}\left[-f'(\xi_+)V_+^2 - f'(\xi_-)V_-^2\right]$, $V_\pm = 2s \pm Z\sqrt{1 - c^2/v_*^2}$, $\xi_\pm = JV_\pm - h$
- only finite if $v_* = ZJb > c \Rightarrow$ no damping in our approximation
- natural explanation for the deviations at larger fields: dilute Bose gas quantum critical point at $B_c = 8.5\,\text{T}$



$r = c/(Jb)$



Research plan

- calculate the correlation functions in the vicinity of the dilute Bose gas quantum critical point by combining the hard-core boson formalism with the functional renormalization group, going beyond the usually used ladder approximation
  $$\mathcal{H}_U = \sum_k(\epsilon_k - \mu)b_k^\dagger b_k + \frac{1}{2N}\sum_{q,k,k'}(J_q + U)b_{k+q}^\dagger b_{k'-q}^\dagger b_{k'}b_k$$
  $$\epsilon_k = J_k^D - J_{\min}^D, \quad \mu = \frac{J_0^D - J_{\min}^D}{2} - h = h_c - h, \quad J_k^D = J_k + D_k$$
  $$J_k = \sum_{\boldsymbol{R}} J(\boldsymbol{R})\cos(\boldsymbol{k}\cdot\boldsymbol{R}), \quad D_k = \sum_{\boldsymbol{R}} D(\boldsymbol{R})\sin(\boldsymbol{k}\cdot\boldsymbol{R})$$
- generalize the hard-core boson formalism to take the coupling of hard-core bosons to the lattice vibrations (phonons) into account
- study ultrasound in the vicinity of the dilute Bose gas quantum critical point and compare with the experiments of B1
- study driven dissipative dilute Bose gas, non-equilibrium time evolution
- connections to projects **B1** **B2** **B3** **B4**

References

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