Nonzero temperature.

Mermin - Wagner theorem

Let us start from quantum ferromagnet.

$$S_n^{(z)} = s - a_n^+ a_n = S - \frac{1}{N} \sum_{k,q} e^{i(\vec{k}-\vec{q})r_n} a_k^+ a_q .$$

$$H = \text{const} + \sum_k \omega_k a_k^+ a_k$$

Density matrix (Gibbs distribution)

$$\rho \propto e^{-H/T} \quad , \quad \rho = \frac{1}{Z} e^{-H/T}$$

$$Z = tr\, e^{-H/T}$$

$$\langle n_k \rangle = tr\left(a_k^+ a_k \rho\right) \longrightarrow tr\left(a^+ a \frac{e^{-\frac{\omega a^+ a}{T}}}{Z}\right)$$

$$Z = tr\, e^{-\frac{\omega a^+ a}{T}} = 1 + e^{-\frac{\omega}{T}} + e^{-\frac{2\omega}{T}} + \dots =$$

$$= \frac{1}{1 - e^{-\omega/T}}$$

$$\langle n\rangle = \frac{1}{Z}\left(e^{-\omega/T} + 2e^{-\frac{2\omega}{T}} + 3e^{-\frac{3\omega}{T}} + \dots\right) =$$

$$= \frac{1}{Z}\left(-\frac{\partial}{\partial x}\right)\underbrace{\left[1 + e^{-\omega/T} + e^{-\frac{2\omega}{T}} + e^{-\frac{3\omega}{T}} + \dots\right]}_{Z}$$

$$x = \omega/T$$

$$\langle \hat{n}\rangle = \frac{1}{Z}\left(-\frac{\partial}{\partial x}\right)Z = -\frac{\partial}{\partial x}\ln Z = \frac{\partial}{\partial x}\left(1-e^{-x}\right) =$$

$$= \frac{e^{-x}}{1-e^{-x}} = \frac{1}{e^{\omega/T}-1}$$ — usual Bose distribution

Thus, in thermal equilibrium

$$\langle a_k^+ a_q\rangle = \delta_{kq}\, n_k \quad , \quad n_k = \frac{1}{e^{\omega_k/T}-1}$$

$$m = \langle S_n^{(z)}\rangle = S - \frac{1}{N}\sum_k n_k = S - \frac{V}{N}\int \frac{d^D k}{(2\pi)^D}\, n_k$$

$\frac{V}{N} = a^D$, a is the lattice spacing.

The magnetization is

$$\boxed{m = S - \int n_k \frac{d^D k}{(2\pi)^D}}$$

— dimensionless momentum $k \to ka$

Start from the 3D case.

$\omega_k = JSk^2$, at small k.

$$m = S - \int \frac{4\pi k^2 dk}{(2\pi)^3} \frac{1}{e^{\frac{JSk^2}{T}} - 1}$$

Here I assume small temperature

$JSk^2 \sim T \Rightarrow k \sim \sqrt{\frac{T}{JS}} \ll \frac{\pi}{a_{=1}} \simeq \pi$

$\Longrightarrow$ $\boxed{T \ll JS}$ in other words T is much smaller than the Curie temperature.

$$m = S - \frac{1}{4\pi^2} \int_0^\infty \frac{k\, dk^2}{e^{\frac{JSk^2}{T}} - 1} = S - \frac{1}{4\pi^2} \left(\frac{T}{JS}\right)^{3/2} \int_0^\infty \frac{\sqrt{x}\, dx}{e^x - 1}$$

$$\int_0^\infty \frac{\sqrt{x}\, dx}{e^x - 1} = \Gamma\left(\tfrac{3}{2}\right) \zeta\left(\tfrac{3}{2}\right) \simeq 2.315$$

Γ-function, Riemann zeta function

Hence

$$\boxed{m = S - \frac{2.315}{4\pi^2} \left(\frac{T}{JS}\right)^{3/2}}$$

2D ferromagnet

$$m = S - \int_0^{\sim 1} \frac{2\pi k\,dk/(2\pi)^2}{e^{\frac{JSk^2}{T}} - 1}$$

The integral is log diverging at $k \to 0$

$\boxed{\text{Hence} \quad m = 0}$ Thermal fluctuations destroy the long range order at any nonzero temperature. Curie temperature is exact zero.

Magnetic order is preserved at the scale of correlation length ξ, $k_{min} \sim \frac{1}{\xi}$

$$\frac{1}{e^{\frac{JSk^2}{T}} - 1} \approx \frac{T}{JSk^2}, \quad \frac{JSk^2}{T} \ll 1 \Leftrightarrow k \lesssim \sqrt{\frac{T}{JS}}$$

$$0 = m = S - \frac{T}{2\pi JS} \int_{1/\xi}^{\sim\sqrt{\frac{T}{JS}}} \frac{dk}{k} = S - \frac{T}{2\pi JS} \ln \xi \sqrt{\frac{T}{JS}}$$

$$\boxed{\xi \sim \sqrt{\frac{JS}{T}}\, e^{\frac{2\pi JS^2}{T}} \longrightarrow e^{\frac{2\pi JS^2}{T}}}$$

1D ferromagnet

$$m = S - \int_0^{\sim \pi/a} \frac{2dk/(2\pi)}{e^{\frac{JSk^2}{T}} - 1}$$

Again the integral is diverging at $k=0$. Hence $m=0$, thermal fluctuations destroy the long range order.

For correlation length we get

$$0 = m = S - \frac{T}{\pi J S} \int_{1/\xi}^{\infty} \frac{dk}{k^2} = S - \frac{T}{\pi J S} \xi$$

$$\boxed{\xi \sim \frac{\pi J S^2}{T}}$$

Summary for ferromagnet.

3D: There is a nonzero Curie temperature.

1D, 2D: There is a long range order only at zero temperature. So the Curie temperature is zero.

Correlation lengths

2D: $\xi \sim e^{\frac{2\pi J S^2}{T}}$, 1D: $\xi \sim \frac{\pi J S^2}{T}$

Antiferromagnet, staggered magnetization

Consider, for example, the sublattice "up":

$$S_n^z = S - a_n^+ a_n = S - \frac{2}{N}\sum_{k,q\in MBZ} e^{i(\bar{k}-\bar{q})\bar{r}_n} a_k^+ a_q =$$

$$= S - \frac{2}{N}\sum_{kq} e^{i(\bar{k}-\bar{q})\bar{r}_n}(u_k\alpha_k^+ + v_k\beta_{-k})(u_q\alpha_q + v_q\beta_{-q}^+)$$

$$m = \langle S_z\rangle = S - \frac{2}{N}\sum_{kq} e^{i(k-q)r_n}\left\langle\left[u_k u_q \alpha_k^+\alpha_q + v_k v_q \beta_{-k}\beta_{-q}^+ + v_k u_q \beta_{-k}\alpha_q + u_k v_q \alpha_k^+\beta_{-q}^+\right]\right\rangle$$

$\beta_{-k}\beta_{-q}^+ = \delta_{kq} + \beta_{-q}^+\beta_{-k}$ – commutator.

In thermal equilibrium

$$\langle \alpha_k^+\alpha_q\rangle = \delta_{kq}\langle\alpha_k^+\alpha_k\rangle = \delta_{kq} n_k$$

$$\langle\beta_{-q}^+\beta_{-k}\rangle = \delta_{kq}\langle\beta_{-k}^+\beta_{-k}\rangle = \delta_{kq} n_{-k}$$

$$\langle\beta_{-k}\alpha_q\rangle = \langle\alpha_k^+\beta_{-q}^+\rangle = 0$$

$$n_k = n_{-k} = \frac{1}{e^{\omega_k/T}-1}$$

Thus

$$m = S - \frac{2}{N}\sum_{k\in MBZ}\left[V_k^2 + (u_k^2 + V_k^2)\,n_k\right]$$

$$\left.\begin{aligned} 2V_k^2 &= \frac{1}{\sqrt{1-\gamma_k^2}} - 1 \\ 2(u_k^2 + V_k^2) &= \frac{2}{\sqrt{1-\gamma_k^2}} \end{aligned}\right\}$$ see page 210

$$\boxed{\begin{aligned} m &= S - \frac{1}{N}\sum_{k}\left\{\left(\frac{1}{\sqrt{1-\gamma_k^2}} - 1\right) + \frac{2n_k}{\sqrt{1-\gamma_k^2}}\right\} = \\ &= S - \int_{k\in MBZ}\left\{\left(\frac{1}{\sqrt{1-\gamma_k^2}} - 1\right) + \frac{2n_k}{\sqrt{1-\gamma_k^2}}\right\}\frac{d^D k}{(2\pi)^D} \end{aligned}}$$

Consider first the zero temperature case

$n_k = 0$

$$m = S - \int_{MBZ} \left(\frac{1}{\sqrt{1-\gamma_k^2}} - 1 \right) \frac{d^D k}{(2\pi)^D}$$

1D: $\gamma_k = \cos k$

2D square: $\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y)$

3D simple cubic: $\gamma_k = \frac{1}{3}(\cos k_x + \cos k_y + \cos k_z)$

small k, $\sqrt{1-\gamma_k^2} \simeq \alpha k$

1D: $$m = S - \int_0^{\frac{\pi}{2a}} \frac{2dk}{2\pi} \left(\frac{1}{\alpha k} - 1 \right)$$

logarithmically divergent at small k.

Hence, the long-range AF order is impossible in 1D even at $T=0$. Quantum fluctuations destroy the order.

2D and 3D antiferromagnets are ok at zero temperature
(2D example – assignment).

$T=0$

$$m = m_0 = S - \frac{1}{N}\sum_K \left\{ \frac{1}{\sqrt{1-\gamma_K^2}} - 1 \right\} =$$

$$= S - \int_{MBZ} \left\{ \frac{1}{\sqrt{1-\gamma_K^2}} - 1 \right\} \frac{d^D K}{(2\pi)^D}, \quad D \geq 2.$$

Nonzero temperature

$$m = m_0 - 2\int \frac{1}{\sqrt{1-\gamma_K^2}} \frac{1}{e^{\omega_K/T}-1} \frac{d^D K}{(2\pi)^D}$$, see page 219.

<u>3D</u>: small T, small K

$$\sqrt{1-\gamma_K^2} \approx \frac{K}{\sqrt{3}}$$

$$\omega_K = 6JS\sqrt{1-\gamma_K^2} \approx cK$$

$c = 2\sqrt{3}SJ$ – magnon speed.

$$m = m_0 - 2\sqrt{3}\int \frac{4\pi k^{\cancel{2}}\,dk}{(2\pi)^3}\,\frac{1}{\cancel{k}}\,\frac{1}{e^{\frac{ck}{T}}-1} =$$

$$= m_0 - \frac{\sqrt{3}}{\pi^2}\left(\frac{T}{c}\right)^2 \int_0^\infty \frac{x\,dx}{e^x-1} = m_0 - \frac{1}{2\sqrt{3}}\left(\frac{T}{c}\right)^2$$

$$\underline{\underline{T \ll c}}$$

integration

$$\int_0^\infty \frac{x^{\alpha-1}\,dx}{e^x-1} = \Gamma(\alpha)\,\zeta(\alpha)$$

γ-function   Riemann zeta function

$$\int_0^\infty \frac{x\,dx}{e^x-1} = \Gamma(2)\,\zeta(2) = \frac{\pi^2}{6}$$

2D antiferromagnet

$$\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y) \simeq 1 - \frac{k^2}{4}, \quad k \ll 1$$

$$\sqrt{1-\gamma_k^2} \simeq \frac{k}{\sqrt{2}}$$

$$\omega_k = 4JS\sqrt{1-\gamma_k^2} \simeq ck$$

$$c = 2\sqrt{2}\,S\,J$$

$$m = m_0 - 2\int \frac{2\pi \cancel{k}\,dk}{(2\pi)^2}\,\frac{\sqrt{2}}{\cancel{k}}\,\frac{1}{e^{ck/T}-1} =$$

$$= m_0 - \frac{\sqrt{2}}{\pi}\int \frac{dk}{e^{ck/T}-1}, \quad \frac{1}{e^{\frac{ck}{T}}-1} \simeq \frac{T}{ck}, \quad k \to 0$$

The integral is log divergent at small k. This means that thermal fluctuations destroy the long-range AF order at any nonzero temperature. The Neel temperature is exact zero.

The antiferromagnetic correlation length ξ.

$$0 = m \approx m_0 - \frac{\sqrt{2}}{\pi}\frac{T}{c}\int_{1/\xi}^{\sqrt{\frac{T}{c}}}\frac{dk}{k} =$$

$$= m_0 - \frac{T}{2\pi J S}\ln \xi\sqrt{\frac{T}{c}}$$

$$\boxed{\xi \sim \sqrt{\frac{c}{T}}\, e^{\frac{2\pi m_0 S J}{T}} \rightarrow e^{\frac{2\pi m_0 S J}{T}}}$$

Summary for antiferromagnets

3D: There is a nonzero Neel temperature

2D: There is AF ordering at $T=0$. However, at $T \neq 0$ thermal fluctuations destroy the order. So, the Neel temperature is zero. The magnetic correlation length $\xi \propto e^{\frac{2\pi m_0 S J}{T}}$

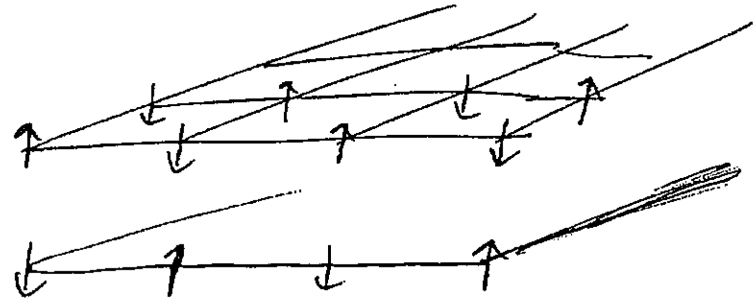
1D: There is ordering even at zero temperature. Quantum fluctuations destroy the order.

O(3) quantum phase transition

Consider an example of two coupled square lattice quantum antiferromagnets with $s = 1/2$

(1)

(2)



$$H = \sum_{\langle ij\rangle} \left[J \vec{S}_i^{(1)} \cdot \vec{S}_j^{(1)} + J \vec{S}_i^{(2)} \vec{S}_j^{(2)} \right] + \sum_i J_\perp \vec{S}_i^{(1)} \vec{S}_i^{(2)}$$

If $J_\perp$ is small, $J_\perp \ll J$, it practically does not influence magnetic dynamics. $J_\perp$ just locks relative magnetization of both planes.

two interacting spins ½ : spin dimer.

$$H = J_\perp \vec{S}_1 \cdot \vec{S}_2$$

$\vec{S} = \vec{S}_1 + \vec{S}_2$ - total spin.

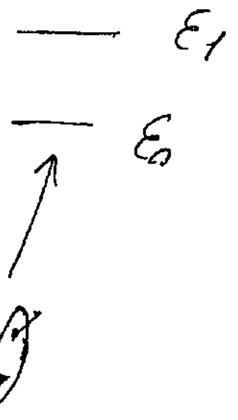
$$S^2 = S_1^2 + S_2^2 + 2\vec{S}_1\vec{S}_2 \Rightarrow \vec{S}_1\cdot\vec{S}_2 = \frac{1}{2}\left[\hat{S}^2 - \frac{3}{4} - \frac{3}{4}\right] =$$

$$= \frac{1}{2}\left[S(S+1) - \frac{3}{2}\right]$$

$$H = \frac{1}{2} J_\perp \left[S(S+1) - \frac{3}{2}\right], \quad S = 0, 1$$

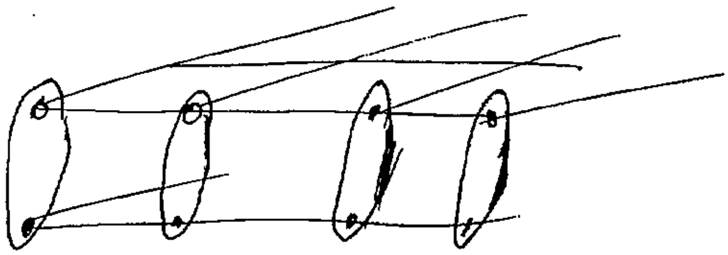
$$\varepsilon_0 = -\frac{3}{4} J_\perp$$

$$\varepsilon_1 = \frac{1}{4} J_\perp$$

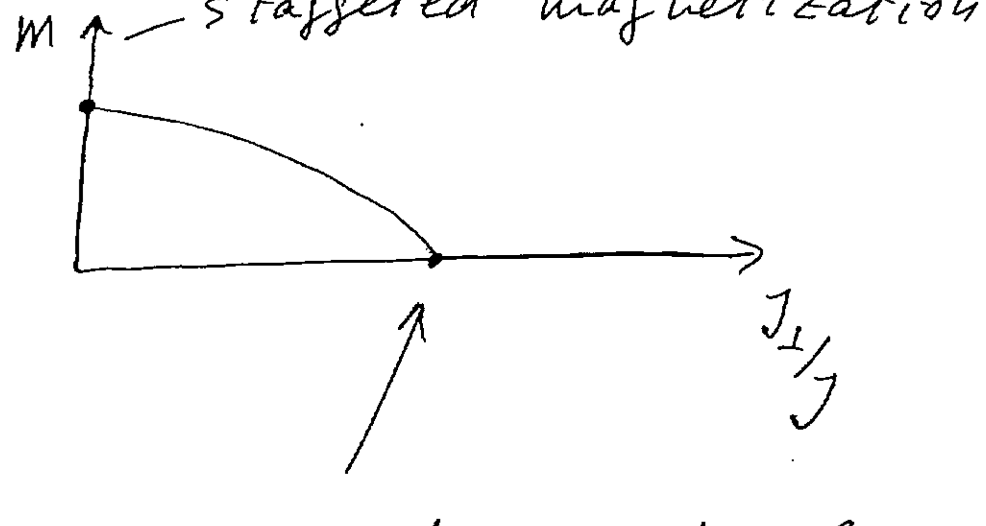


$$|S=0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2\right).$$

Two coupled Heisenberg planes in the limit $J_\perp \gg J$ consist of set of spin dimers



There is no staggered magnetization in this state



numerics (quantum Monte Carlo) shows that the QCP is located at $\frac{J_\perp}{J} \approx 2.52$

Quantum field theory describing the QCP.

The vector field $\vec{\varphi}$ describes the staggered magnetization

$\vec{m} \propto \vec{\varphi}$

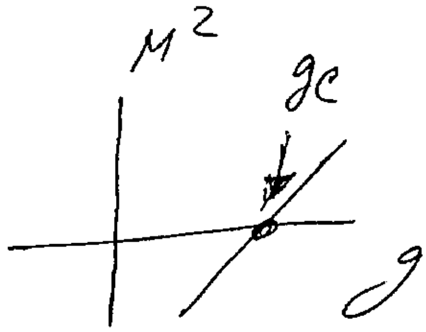
$$\mathcal{L} = \frac{1}{2}\dot{\vec{\varphi}}^2 - \frac{c^2}{2}(\vec{\nabla}\vec{\varphi})^2 - \frac{M^2}{2}\vec{\varphi}^2 - \frac{\alpha}{4}(\vec{\varphi}^2)^2$$

The Lagrangian describing dynamics of the field $\vec{\varphi}$ (density of Lagrangian)

Landau–Ginzburg–Wilson paradigm

Assume that M^2 depends on some external parameter g ("the coupling constant"). In the above example of two Heisenberg planes, $g = J_\perp / J$. In the experimental example which I will discuss later, g is external preassure.

(A) $M^2(g) = \lambda^2 (g - g_c)$



g_c is the critical value of the coupling constant.

Remind Euler – Lagrange eqs.

$$\frac{\partial}{\partial t}\frac{\delta \mathcal{L}}{\delta \dot{\vec{\varphi}}} = \frac{\delta \mathcal{L}}{\delta \vec{\varphi}}$$

$$E = \dot{\vec{\varphi}}\frac{\delta \mathcal{L}}{\delta \dot{\vec{\varphi}}} - \mathcal{L}$$ – energy density

$$E = \dot{\vec{\varphi}}^2 - \frac{1}{2}\dot{\vec{\varphi}}^2 + \frac{c^2}{2}(\nabla\vec{\varphi})^2 + \frac{M^2}{2}\vec{\varphi}^2 + \frac{\alpha}{4}\vec{\varphi}^4 =$$

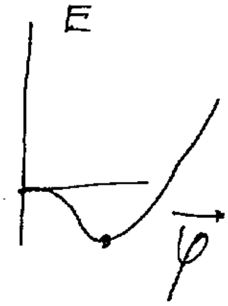
$$= \frac{1}{2}\dot{\vec{\varphi}}^2 + \frac{c^2}{2}(\nabla\vec{\varphi})^2 + \frac{M^2}{2}(\vec{\varphi})^2 + \frac{\alpha}{4}\vec{\varphi}^4$$

Ground state corresponds to a constant solution, $\vec{\varphi} = \vec{\varphi}_0 = \text{const}$.

Ground state has to minimize energy

1) If $M^2 > 0$ then $\vec{\varphi}_0 = 0$,

2) If $M^2 < 0$

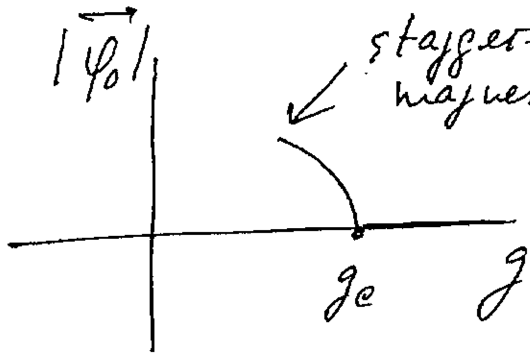


Spontaneous violation of the O(3) symmetry

then

$$\vec{\varphi}_0^{\,2} = \left(\frac{\alpha}{|M|^2}\right)^{-1} = \frac{\lambda^2 (g_c - g)}{\alpha}$$

$$|\vec{\varphi}_0| = \frac{\lambda}{\sqrt{\alpha}} \sqrt{g_c - g}$$



Excitation spectrum, $\boxed{\dfrac{\partial}{\partial t} \dfrac{\delta \mathcal{L}}{\delta \dot{\vec{\varphi}}} = \dfrac{\delta \mathcal{L}}{\delta \vec{\varphi}}}$

$$\frac{\delta \mathcal{L}}{\delta \dot{\vec{\varphi}}} = \dot{\vec{\varphi}}$$

$$\frac{\delta \mathcal{L}}{\delta \vec{\varphi}} = c^2 \Delta \vec{\varphi} - M^2 \vec{\varphi} - \alpha (\vec{\varphi})^2 \vec{\varphi}$$

Hence

$$\boxed{\ddot{\vec{\varphi}} - c^2 \Delta \vec{\varphi} + M^2 \vec{\varphi} + \alpha \vec{\varphi}^{\,2} \vec{\varphi} = 0}$$

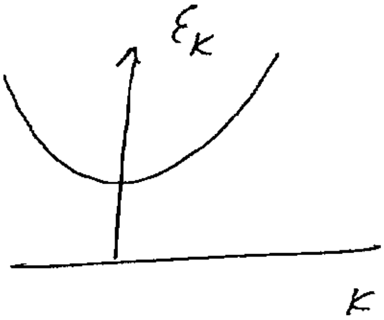
1) Symmetric phase, $g > g_c \Leftrightarrow M^2 > 0$, there is no a spontaneous violation, no staggered magnetization

$$\vec{\varphi}^2 \to \vec{\varphi}_0^{\,2} = 0 \quad \text{- ground state.}$$

$$\ddot{\vec{\varphi}} - c^2 \Delta \vec{\varphi} + M^2 \vec{\varphi} = 0$$

$$\vec{\varphi} = \vec{a}\, e^{-i\omega t + i\vec{k}\vec{r}}$$

$$\omega_k = \sqrt{M^2 + c^2 k^2}$$



a) there is a gap in the excitation spectrum

б) there are 3 degenerate polarizations

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2) Spontaneously broken phase, $g < g_c \Leftrightarrow M^2 < 0$. there is a nonzero staggered magnetization

$$\varphi_0, \quad |\varphi_0|^2 = \left(\frac{\alpha}{|M|^2}\right)^{-1} = \frac{\lambda^2 (g_c - g)}{\alpha}$$

Excitations with polarization perpendicular to the direction of the staggered magnetization $\vec{\varphi_0}$

$$\vec{\varphi} = \vec{\varphi_0} + \delta\vec{\varphi_\perp} \qquad \vec{\varphi_0}\cdot\delta\vec{\varphi_\perp} = 0$$

Eq. of motion follows from that in page 230

$$\delta\ddot{\vec{\varphi}}_\perp - c^2\Delta\delta\vec{\varphi}_\perp + \underbrace{(M^2 + 2\vec{\varphi_0}^2)}_{\parallel \atop 0 \text{ — see page } 230}\delta\vec{\varphi}_\perp = 0$$

$$\boxed{\delta\ddot{\vec{\varphi}}_\perp + c^2\Delta\delta\vec{\varphi}_\perp = 0}$$

$$\delta\vec{\varphi}_\perp = \vec{a}_\perp e^{-i\omega t + i\vec{k}\vec{r}}$$

$$\omega = ck$$

The spectrum is gapless and linear in k

There are two independent polarizations

These are magnons in AF which we derived at page 49 using different techniques.

The magnons are gapless in accordance with Goldstone theorem.

Longitudinal magnon:

$\delta\vec{\varphi}$ is parallel to $\vec{\varphi_0}$

$$\vec{\varphi} = \vec{\varphi_0} + \delta\vec{\varphi_\parallel}$$

Again, use eq. of motion at page 23C

$$0 = \delta\ddot{\vec{\varphi}}_\parallel - c^2 \Delta \delta\varphi_\parallel + M^2(\delta\vec{\varphi}_\parallel + \vec{\varphi_0}) + \alpha(\vec{\varphi_0} + \delta\vec{\varphi}_\parallel)^2(\vec{\varphi_0} + \delta\vec{\varphi}_\parallel)$$

$$= \delta\ddot{\vec{\varphi}}_\parallel - c^2 \Delta \delta\vec{\varphi}_\parallel + (\vec{\varphi_0} + \delta\vec{\varphi}_\parallel)\underbrace{\left[M^2 + \alpha\vec{\varphi_0}^2\right]}_{=0} +$$

$$+ \alpha 2 \varphi_0^2 \delta\varphi_\parallel + \cancel{O(\delta\varphi_\parallel^2)}$$

$$\boxed{\delta\ddot{\vec{\varphi}}_\parallel - c^2 \Delta \delta\vec{\varphi}_\parallel + 2|M^2|\delta\varphi_\parallel = 0}$$

$$2|M^2| = 2\alpha\varphi_0^2 = 2\lambda^2(g_c - g)$$

$$\delta\vec{\varphi}_\parallel = \vec{a}_\parallel e^{-i\omega t + ikr}$$

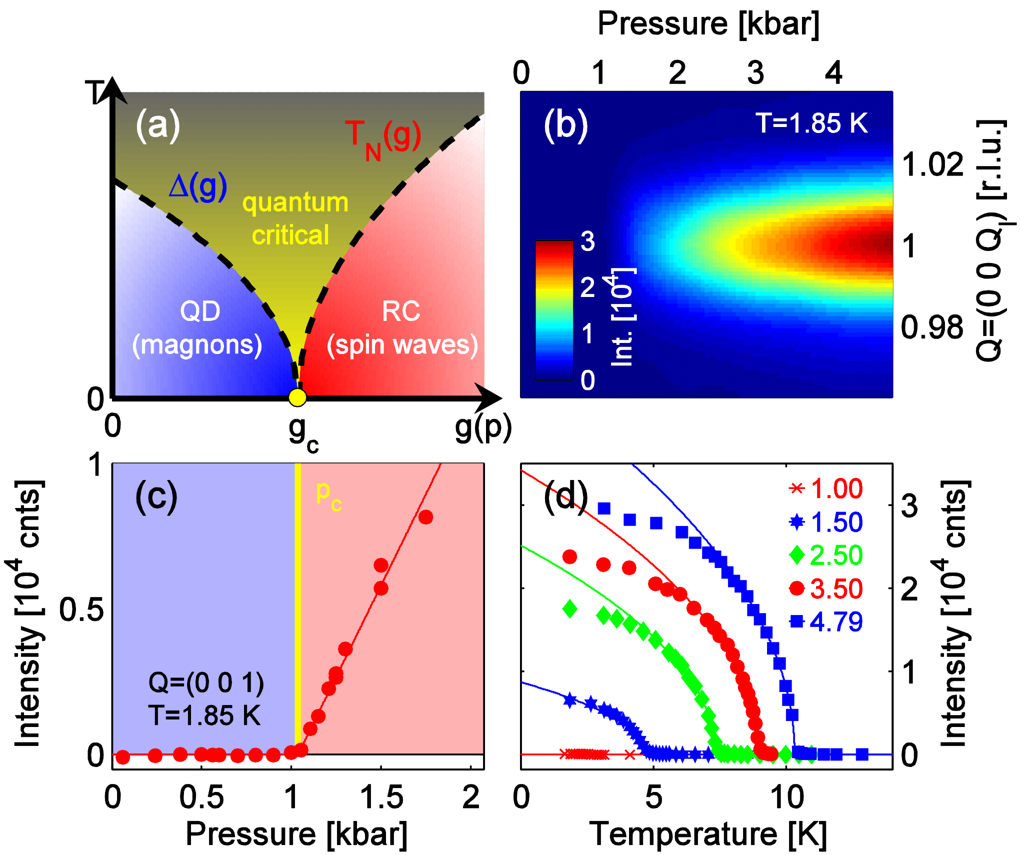
$$\omega = \sqrt{2|M^2| + c^2k^2}$$

The longitudinal mode is gapped

$$\Delta = \sqrt{2|M^2|} = \sqrt{2}\lambda(g_c - g).$$

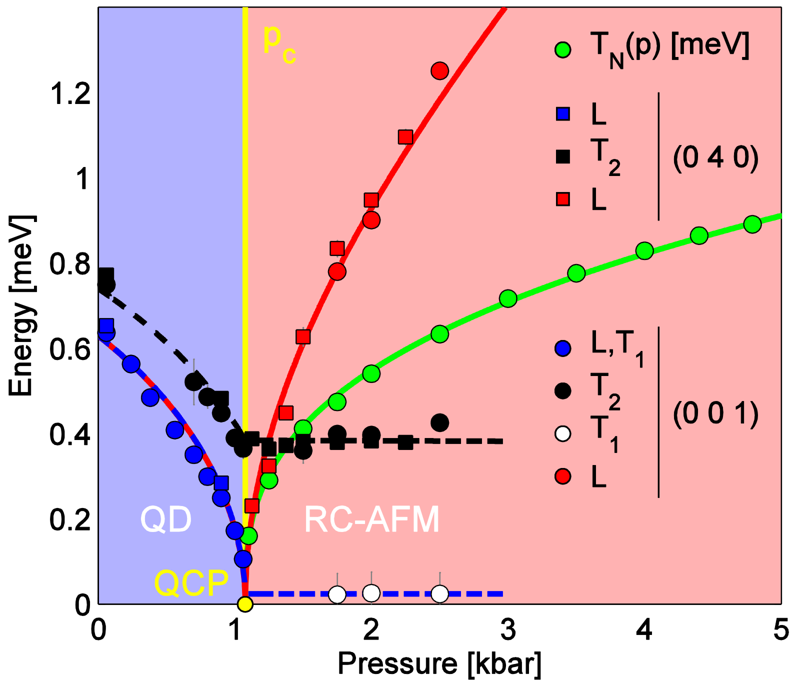
Pressure induced O(3) magnetic quantum phase transition (QPT) in $TlCuCl_3$

Ruegg, et al, Phys. Rev. Lett. **100**, 205701 (2008).



(a) The phase diagram for a QPT driven by preassure.

(b–d) Pressure– and temperature–dependence of the neutron scattering magnetic Bragg peak intensity at Q = (0 0 1) which is proportional to the square of the order parameter m, the square of the staggered magnetization. Compare Fig.c with Eq. (A) on page 67.



Magnetic excitations gaps measured by inelastic neutron scattering.
Blue circles on the left show the gap in the magnetically disordered phase,
White circles on the right show the gapless Goldstone mode in the antiferromagnetic phase.
Red circles/squares on the right show the gapped longitudinal mode in the antiferromagnetic phase.

Compare the experimental data with predictions of theory on pages 69-71.