

7 Magnetic quantum phase transitions

7.1 Order parameters and response functions

Local order parameter ψ :

$$\langle \hat{O}(\vec{R}) \rangle = \text{Re} \left[e^{i\vec{Q} \cdot \vec{R}} \psi(\vec{R}) \right]$$

where $\psi(\vec{R})$ a slowly varying function of \vec{R} , can be scalar, vector, tensor, etc., $\hat{O}(\vec{R})$ a local observable, and \vec{Q} the ordering wavevector, with $e^{i\vec{Q} \cdot \vec{R}}$ chosen such that it captures (possible) fast oscillations in \hat{O}

Examples:

- Charge density wave (CDW):

$$\langle \hat{S}(\vec{R}) \rangle = S_0 + \text{Re} \left[e^{i\vec{Q} \cdot \vec{R}} \psi_c(\vec{R}) \right]$$

↑ charge-density operator
↑ average charge density
↑ scalar with N=1 components

- Spin density wave (SDW):

$$\langle \hat{S}(\vec{R}) \rangle = \text{Re} \left[e^{i\vec{Q} \cdot \vec{R}} \vec{\psi}_s(\vec{R}) \right]$$

↑ vector with N=3 components

E.g., square-lattice AFM with $\vec{Q} = \frac{\vec{b}_1 + \vec{b}_2}{2} = \left(\frac{\pi}{a}, \frac{\pi}{a}\right)$ and $\vec{\psi}_s$ the "staggered magnetization" reciprocal lattice vectors

Remarks:

- $\vec{Q}=0 \Rightarrow \Psi$ real (for Hermitian \hat{O})
- \vec{Q} finite with $\vec{Q} \neq \sum_{i=1}^d \frac{n_i}{2} \vec{b}_i \Rightarrow \Psi$ complex
- Phase of complex Ψ discrete for commensurate \vec{Q} (i.e., for $\vec{Q} = \sum q_i \vec{b}_i$ with $q_i \in \mathbb{Q}$)

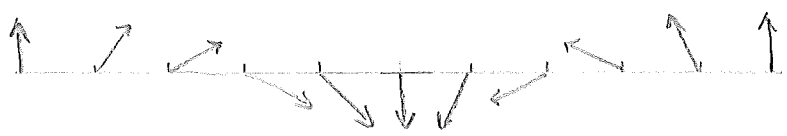
Classes of spin density waves (vector orders):

- Collinear: $\langle \vec{S}_i \rangle \parallel \vec{n}$ for all $i \Rightarrow \vec{\Psi}_S(\vec{R}) = e^{i\theta(\vec{R})} \vec{n}$

"sliding degree of freedom"



- Spiral: $\vec{\Psi} = \vec{n}_1 + i\vec{n}_2$ with $\vec{n}_1 \cdot \vec{n}_2 = 0, \vec{n}_1, \vec{n}_2 \in \mathbb{R}^3$



Real-time correlation function (measurable, e.g., in neutron scattering):

$$C(\vec{r}, t; \vec{r}', t') = \langle \hat{\Psi}(\vec{r}, t) \hat{\Psi}(\vec{r}', t') \rangle$$

Dynamic structure factor:

$$S(\vec{K}, \omega) = \int d^d \vec{r} \int_{-\infty}^{\infty} dt C(\vec{r}, t; 0, 0) e^{-i\vec{K} \cdot \vec{r} + i\omega t}$$

assuming translational invariance $C(\vec{r}, t; \vec{r}', t') \equiv C(\vec{r}-\vec{r}', t-t'; 0, 0)$.

Imaginary-time correlation function:

$$C(\vec{r}, \tau; \vec{r}', \tau') = \left\langle \hat{T}_\tau \left[\hat{\psi}(\vec{r}, \tau) \hat{\psi}(\vec{r}', \tau') \right] \right\rangle$$

$$\text{where } \hat{T}_\tau [\hat{A}(\tau) \hat{B}(\tau')] = \begin{cases} \hat{A}(\tau) \hat{B}(\tau') & \text{if } \tau > \tau' \\ \hat{B}(\tau') \hat{A}(\tau) & \text{if } \tau < \tau' \end{cases}$$

Dynamic susceptibility:

$$\chi(\vec{k}, i\omega_n) = \int d^d \vec{r} \int_0^\beta d\tau C(\vec{r}, \tau; 0, 0) e^{-i\vec{k} \cdot \vec{r} + i\omega_n \tau}$$

with the (bosonic) Matsubara frequencies $\omega_n = 2\pi nT$, $n = 0, \pm 1, \pm 2, \dots$

Fluctuation-dissipation theorem:

$$S(\vec{k}, \omega) = \frac{2}{1 - e^{-\omega/T}} \text{Im} \chi(\vec{k}, \omega)$$

\uparrow "fluctuation" \nwarrow "dissipation"

with $\text{Im} \chi(\vec{k}, \omega)$ "spectral density" (from analytic continuation $i\omega_n \leftrightarrow \omega + i\delta \Big|_{\delta \rightarrow 0}$)

7.2 Properties of the quantum ϕ^4 model

Action:

$$S = \int d^d \vec{r} \int_0^\beta d\tau \left(\frac{c^2}{2} (\nabla \phi)^2 + \frac{1}{2} (\partial_\tau \phi)^2 + \frac{\tau}{2} \phi^2 + \frac{u}{4!} \phi^4 \right)$$

Zero-temperature properties:

- Dynamic exponent $z=1$

- Quantum-to-classical correspondence: $QCP(d) \cong TCP(d+1)$

thermal critical point
 \downarrow
 in $d+z=d+1$ dimensions

\uparrow
 additional imaginary
 time direction

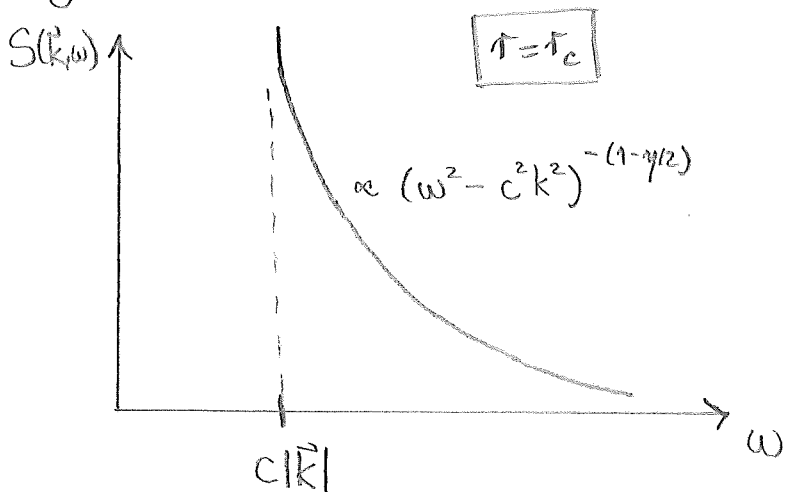
- Critical two-point correlator:

$$\chi(\vec{k}, \omega) \propto \frac{1}{(c^2 \vec{k}^2 - (\omega + i\delta)^2)^{\frac{2-\eta}{2}}}$$

"critical continuum
of excitations"

with $\omega + i\delta \Big|_{\delta \rightarrow 0} \leftrightarrow i\omega_n$

- Dynamic structure factor $S(\vec{k}, \omega) \propto \text{Im} \chi(\vec{k}, \omega)$:



No quasiparticle excitations for $\eta \neq 0$!

Disordered phase ($\tau > \tau_c$):

$$S(\vec{k}, \omega) \propto \text{Im} \chi(\vec{k}, \omega) = \text{Im} \left[\frac{1}{c^2 k^2 + \tau - (\omega + i\delta)^2 - \Sigma(\vec{k}, \omega)} \right]$$

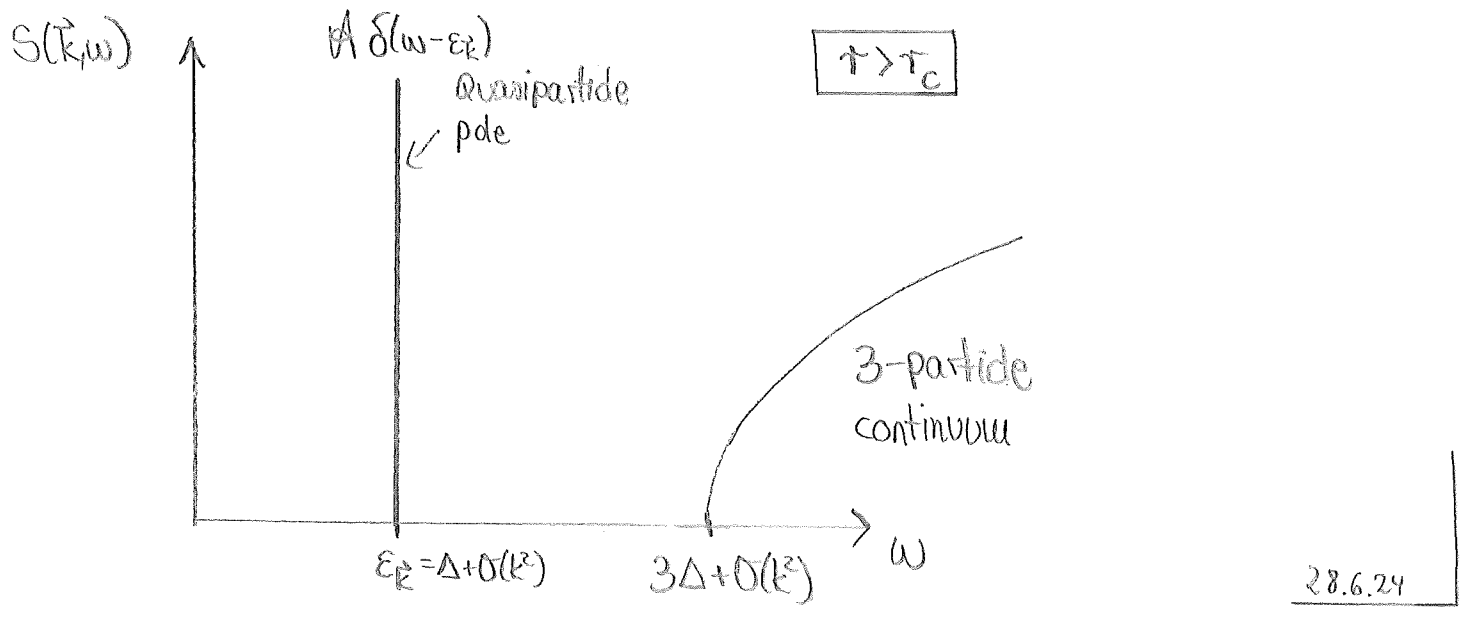
↑ from $\frac{n}{4!} \phi^4$ self-interaction

$$= \frac{A}{2\varepsilon_{\vec{k}}} \left[\delta(\omega - \varepsilon_{\vec{k}}) - \delta(\omega + \varepsilon_{\vec{k}}) \right] \quad (\text{small } \omega)$$

with quasiparticle dispersion $\varepsilon_{\vec{k}}^2 = c^2 k^2 + \tau - \Sigma$ and quasiparticle pole A .

Remarks:

- Self-energy Σ modifies $\varepsilon_{\vec{k}}$ and A , but does not remove the quasiparticle pole
- Energy gap $\Delta = \sqrt{\tau - \Sigma(\vec{k}=0, \omega=\Delta)}$ $\hat{=}$ frequency of quasiparticle pole at $\vec{k}=0$
- Dispersion near $k=0$: $\varepsilon_{\vec{k}} = \Delta + \frac{c^2}{2\Delta} k^2 + O(k^4)$
- Higher energies $\omega > n \cdot \Delta$, $n = 3, 5, 7, \dots$: n -particle continua from scattering processes



Limit $\tau \searrow \tau_c$:

$$\chi(\vec{k}, \omega) = \frac{1}{\Delta^{2-\eta}} f_x\left(\frac{ck}{\Delta}, \frac{\omega}{\Delta}\right) \quad \text{scaling form}$$

\Rightarrow scaling of single-particle pole: $A \propto \Delta^z \propto (\tau - \tau_c)^{2\nu} \quad (z=1)$

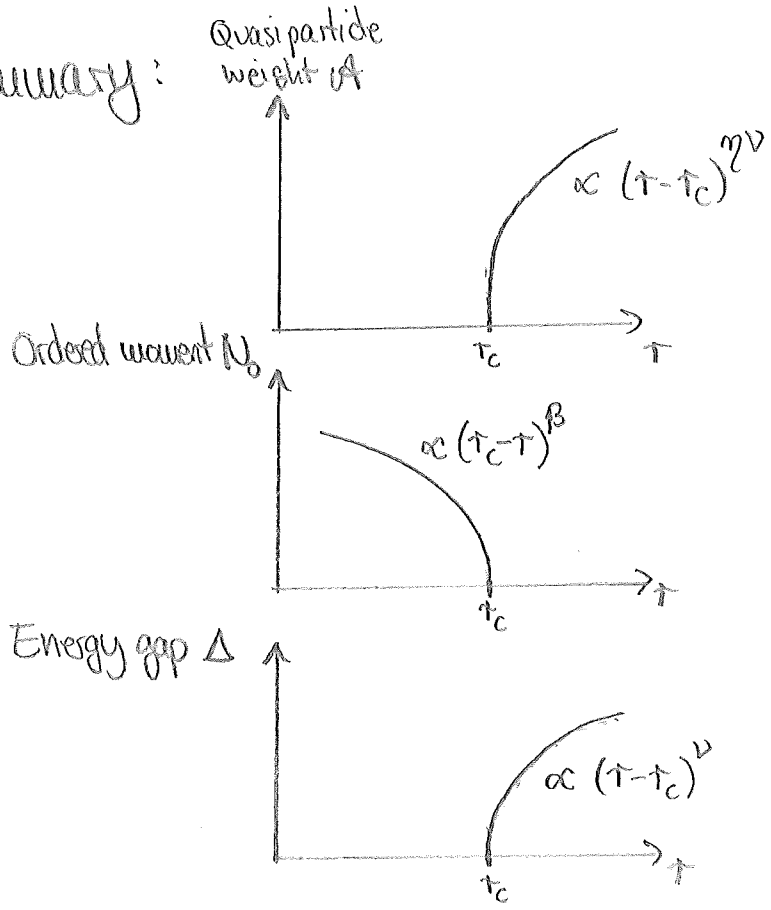
Ordered phase ($\tau < \tau_c$):

$$S(\vec{k}, \omega) = N_0^2 (2\pi)^{d+1} \delta(\omega) \delta(\vec{k}) + O(\omega) \quad \begin{array}{l} \uparrow \\ \text{order parameters} \end{array} \quad \begin{array}{l} \text{"Bragg peak"} \\ \text{at } \vec{k}=0 \end{array}$$

Susceptibility ($N > 1$):

- Transverse susceptibility χ_{\perp} : poles at $\omega=0$ "Goldstone modes"
- Longitudinal susceptibility χ_{\parallel} : poles at $\omega \neq 0$ "Higgs mode" ("amplitude mode")

Summary:



7.3 Quantum Ising chain

Hamiltonian:

$$H_I = -J \sum_{i=1}^M (g \sigma_i^x + \sigma_i^z \sigma_{i+1}^z)$$

Strong-coupling limit $g \gg 1$

Ground state:

- $g = \infty$: $|\Psi_0\rangle = \prod_i |\rightarrow\rangle_i$ with $\sigma_i^x |\rightarrow\rangle_i = +|\rightarrow\rangle_i$
"polarized state"

- $g < \infty$: $|\Psi_0\rangle = \prod_i |\rightarrow\rangle_i - \frac{1}{2g} \sum_i |\rightarrow_1 \dots \rightarrow_{i-1} \leftarrow_i \leftarrow_{i+1} \rightarrow_{i+2} \dots \rightarrow_n\rangle + O(\frac{1}{g^2})$

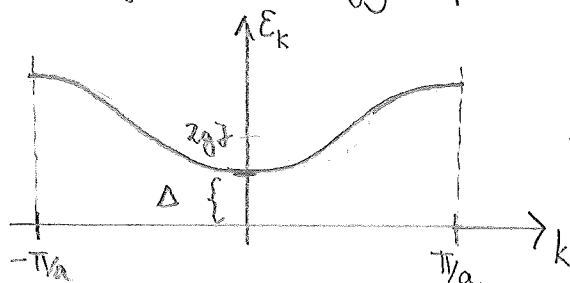
since $\sigma_i^z |\rightarrow\rangle_i = |\leftarrow\rangle_i$ "spin-flip operator"

\Rightarrow correlation-function $C(x,0) \sim e^{-x/g}$ (disordered phase)

One-particle excitations:

- $g = \infty$: First excited state $|i\rangle = |\leftarrow\rangle_i \prod_{j \neq i} |\rightarrow\rangle_j$ with energy $\epsilon = 2gJ$

- $g < \infty$: $|k\rangle = \frac{1}{\sqrt{N}} \sum_j e^{ikj} |j\rangle$ with energy dispersion $\epsilon_k = gJ (2 - \frac{2}{g} \cos ka + O(\frac{1}{g^2}))$



$$\Delta = 2J(g-1) + O(\frac{1}{g})$$

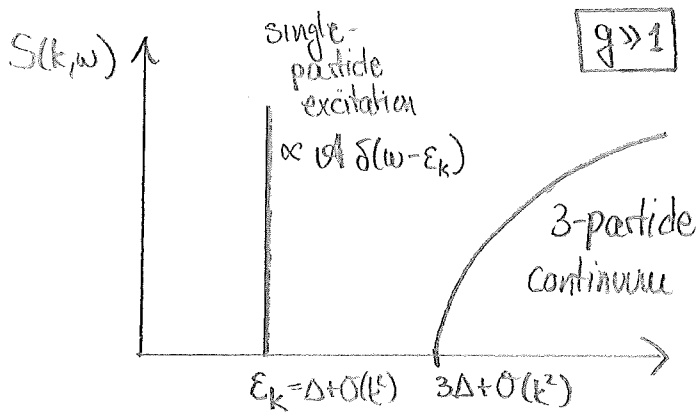
Two-particle excitations:

- $g = \infty$: $|ij\rangle = |\leftarrow\rangle_i |\leftarrow\rangle_j \prod_{l \neq i,j} |\rightarrow\rangle_l$
- $g < \infty$: superposition of $|k_1\rangle$ and $|k_2\rangle$ for i,j far apart with $E_k = E_{k_1} + E_{k_2}$ and $k = k_1 + k_2$

Dynamic structure factor ($T=0$):

$$S(k, \omega) = 2\pi \sum_{|\Psi_\alpha\rangle} |\langle \Psi_\alpha | \sigma^z | \Psi_0 \rangle|^2 \delta(\omega - E_\alpha)$$

↑
energy eigenstates



Correlation function:

$$\lim_{|x| \rightarrow \infty} C(x, 0) = N_0^2 \neq 0 \quad (\text{ordered phase})$$

Ground state:

• $g=0$:

$$|\Psi_0\rangle = \begin{cases} \prod_i |\uparrow\rangle_i \\ \prod_i |\downarrow\rangle_i \end{cases}$$

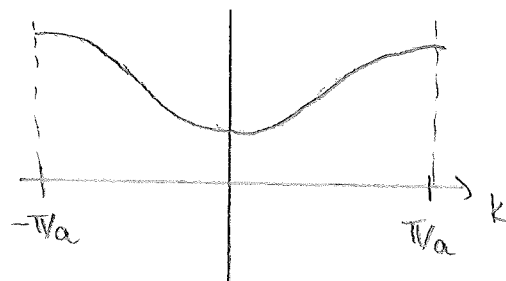
• $g>0$:

$$|\Psi_0\rangle = \begin{cases} \prod_i |\uparrow\rangle_i - \frac{g}{2} \sum_i |\dots \uparrow \downarrow_i \uparrow \uparrow \dots\rangle + O(g^2) \\ (\uparrow \leftrightarrow \downarrow) \end{cases}$$

One-particle excitations:

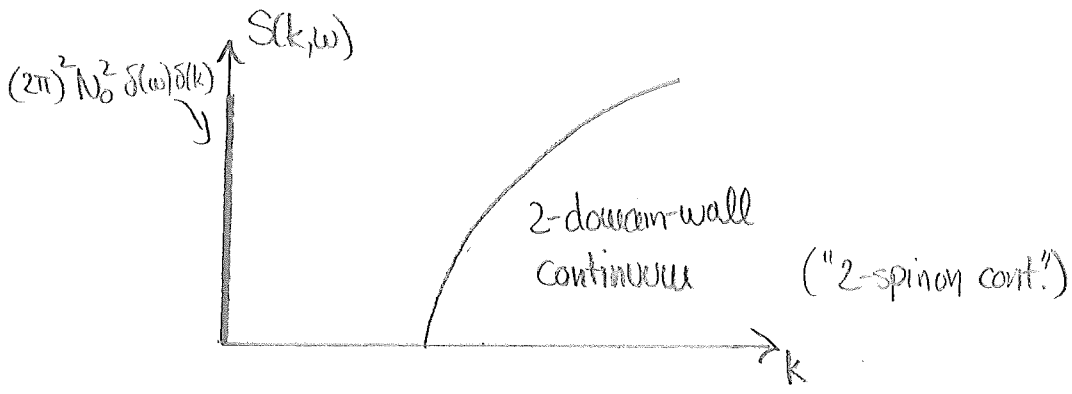
• $g=0$: $|i\rangle = |\dots \uparrow \downarrow_i \downarrow \downarrow \dots\rangle$ with $\epsilon = 2J$ (domain wall at i)

• $g>0$: $|k\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ikx_i} |i\rangle$ with $\epsilon_k = J(2 - 2g \cos ka) + O(g^2)$



Dynamic structure factor:

- Bragg peak at $k=0$ and $\omega=0$ (ordered phase)
- No one-particle peak, since domain walls can only be created in pairs (1D)



Exact spectrum

Jordan-Wigner transformation:

$$\sigma_i^z = 1 - 2 c_i^+ c_i$$

$$\sigma_i^+ = \prod_{j < i} (1 - 2 c_j^+ c_j) c_i$$

$$\sigma_i^- = \prod_{j < i} (1 - 2 c_j^+ c_j) c_i^+$$

with $\sigma_i^\pm = \sigma_i^x \pm i \sigma_i^y$ and $\{c_i, c_j^+\} = \delta_{ij}$ fermions

Inverse transformation:

$$c_i = \left(\prod_{j < i} \sigma_j^z \right) \sigma_i^+$$

$$c_i^+ = \left(\prod_{j < i} \sigma_j^z \right) \sigma_i^-$$

Quantum Ising chain ($\sigma^x \leftrightarrow \sigma^z$):

(84)

$$H_I = -J \sum_i \left[(c_i + c_i^\dagger)(1 - 2c_i^\dagger c_i)(c_{i+1} + c_{i+1}^\dagger) + g(1 - 2c_i^\dagger c_i) \right]$$

$$= -J \sum_i \left(c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i + c_{i+1}^\dagger c_i - 2g c_i^\dagger c_i + g \right)$$

1.7.24

Fourier transformation:

$$H_I = J \sum_k \left[2(g - \cos(ka)) c_k^\dagger c_k - i \sin(ka) (c_{-k}^\dagger c_{-k}^\dagger + c_{-k} c_k) - g \right]$$

Bogoliubov transformation:

$$\gamma_k = u_k c_k - i v_k c_k^\dagger \quad \Leftrightarrow \quad c_k = u_k \gamma_k + i v_k \gamma_{-k}^\dagger$$

with $u_k^2 + v_k^2 = 1 \Leftrightarrow u_k = \cos \frac{\theta_k}{2}$ and $v_k = \sin \frac{\theta_k}{2}$

For
$$\tan \theta_k = \frac{\sin ka}{\cos ka - g}$$

the Hamiltonian becomes diagonal in $\gamma_k, \gamma_k^\dagger$:

$$H_I = \sum_k \epsilon_k \left(\gamma_k^\dagger \gamma_k - \frac{1}{2} \right)$$

with dispersion:

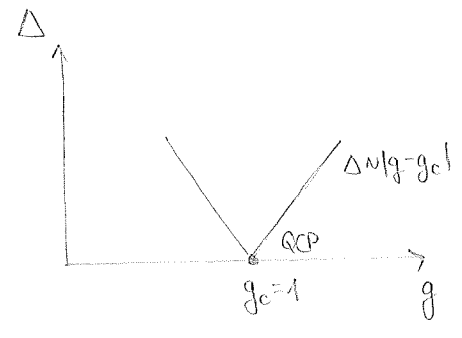
$$\epsilon_k = 2J \sqrt{1 + g^2 - 2g \cos ka} \geq 0$$

Band gap:

$$\Delta = \epsilon_{k=0} = 2J |1-g| = 0 \Leftrightarrow g = g_c = 1$$

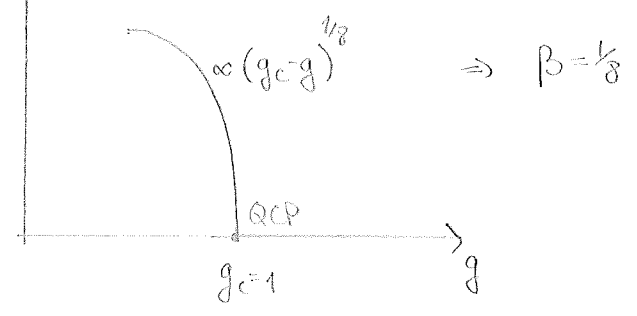
Critical behavior

$$\Delta \propto \frac{1}{\tau_c} \propto \left(\frac{1}{\xi}\right)^2 \propto |g-g_c|^{0.2} \Rightarrow \nu z = 1$$

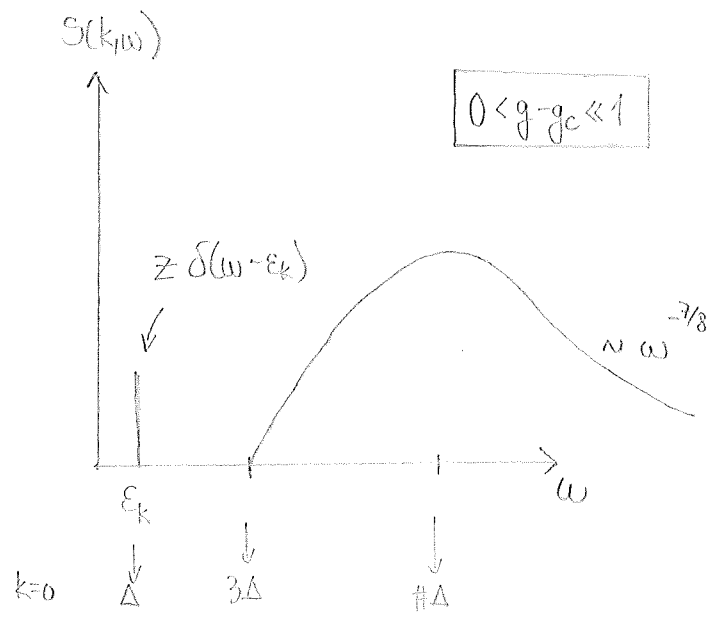
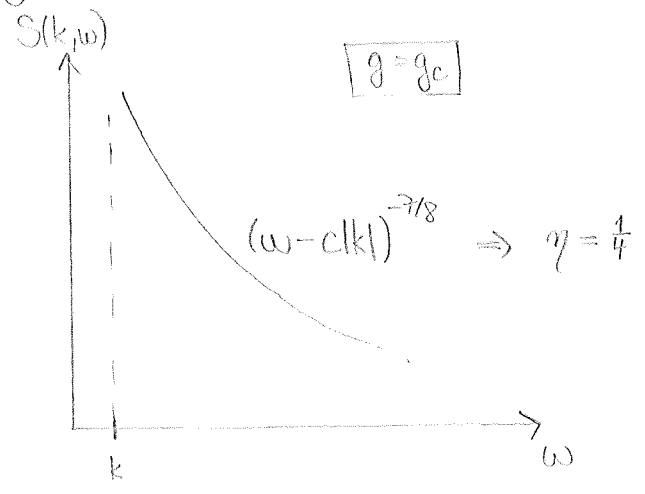


Further results (from exact solution):

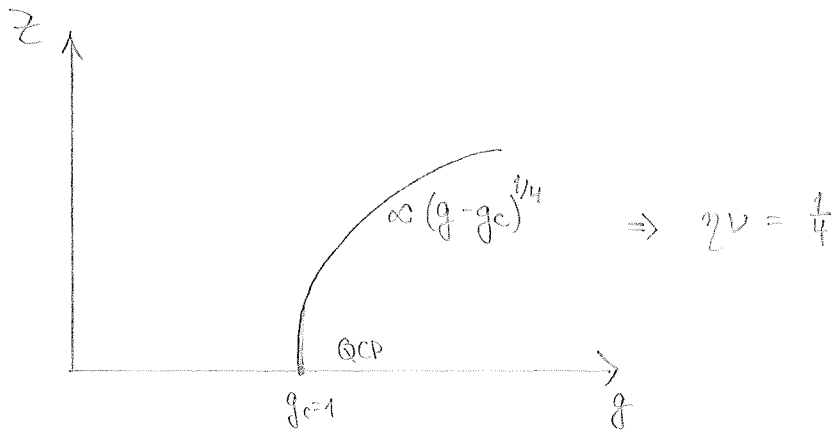
Order parameter: N_0



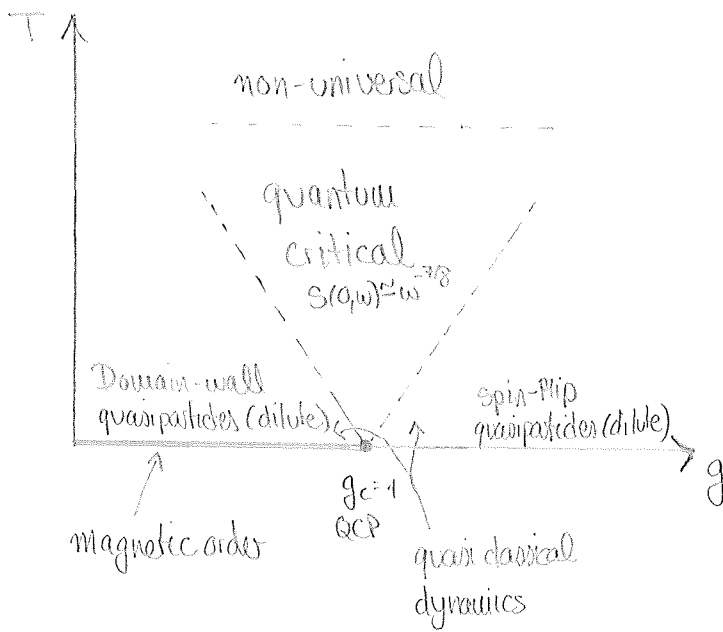
Dynamic structure factor:



Flipped-spin quasiparticle weight ($g > g_c$):



Finite-temperature phase diagram:



Critical exponents:

$$\left. \begin{aligned} \nu &= 1 \\ \eta &= \frac{1}{4} \\ \beta &= \frac{1}{8} \\ z &= 1 \end{aligned} \right\} \text{classical 2D Ising universality class}$$