7 Magnetic quantum phase transitions

7.1 Order parameters and response functions

Local order parameter φ:

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

where $\varphi(\vec{R})$ 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 wavector, with $e^{i\vec{Q}\cdot\vec{R}}$ chosen such that it captures (possible) fast oscillations in $\hat{O}$

Examples:

- Charge density wave (CDW):

$$\langle \underbrace{\hat{\rho}(\vec{R})}_{\text{charge-density operator}} \rangle = \underbrace{\rho_0}_{\text{average charge density}} + \mathrm{Re}\left[e^{i\vec{Q}\cdot\vec{R}} \underbrace{\varphi_c(\vec{R})}_{\text{scalar with } N=1 \text{ components}} \right]$$

- Spin density wave (SDW):

$$\langle \hat{\vec{S}}(\vec{R}) \rangle = \mathrm{Re}\left[e^{i\vec{Q}\cdot\vec{R}} \underbrace{\vec{\varphi}_s(\vec{R})}_{\text{vector with } N=3 \text{ components}} \right]$$

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

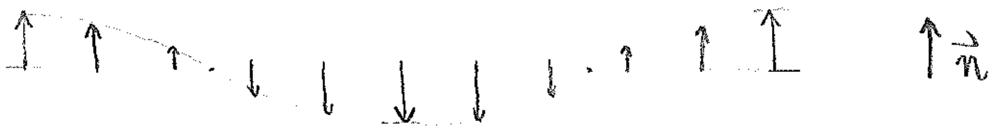
Remarks:

- $\vec{Q}=0 \Rightarrow \varphi$ real (for Hermitean $\hat{O}$)
- $\vec{Q}$ finite with $\vec{Q} \neq \sum_{i=1}^{d} \frac{n_i}{2}\vec{b}_i \Rightarrow \varphi$ complex
- Phase of complex φ discrete for <u>commensurate</u> $\vec{Q}$ (i.e., for $\frac{|\vec{Q}|}{a} \in \mathbb{Q}$)

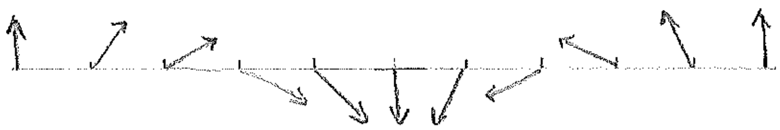
Classes of spin density waves (vector orders):

"sliding degree of freedom"

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



- Spiral: $\vec{\varphi} = \vec{n}_1 + i\vec{n}_2$ 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):

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

Dynamic structure factor:

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

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

Imaginary-time correlation function:

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

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

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 $\omega_n = 2\pi n T$, $n = 0, \pm 1, \pm 2, \dots$

Fluctuation-dissipation theorem:

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

"fluctuation" "dissipation"

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

7.2 Properties of the quantum ϕ^4 model

Action:

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

Zero-temperature properties:

- Dynamic exponent $z = 1$
- Quantum-to-classical correspondence: $QCP(d) \hat{=} TCP(d+1)$

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

  additional imaginary time direction

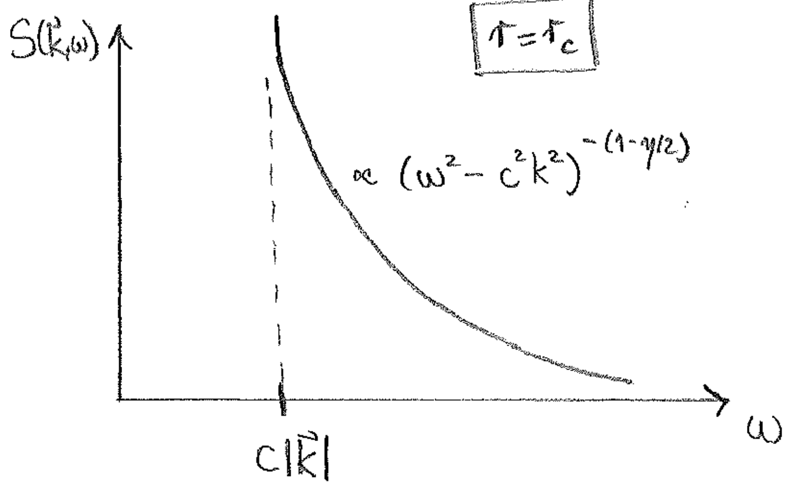
- Critical two-point correlator:

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

"critical continuum of excitations"

with $\omega + i\delta\big|_{\delta\to 0} \leftrightarrow i\omega_n$

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



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

Disordered phase ($r > r_c$):

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

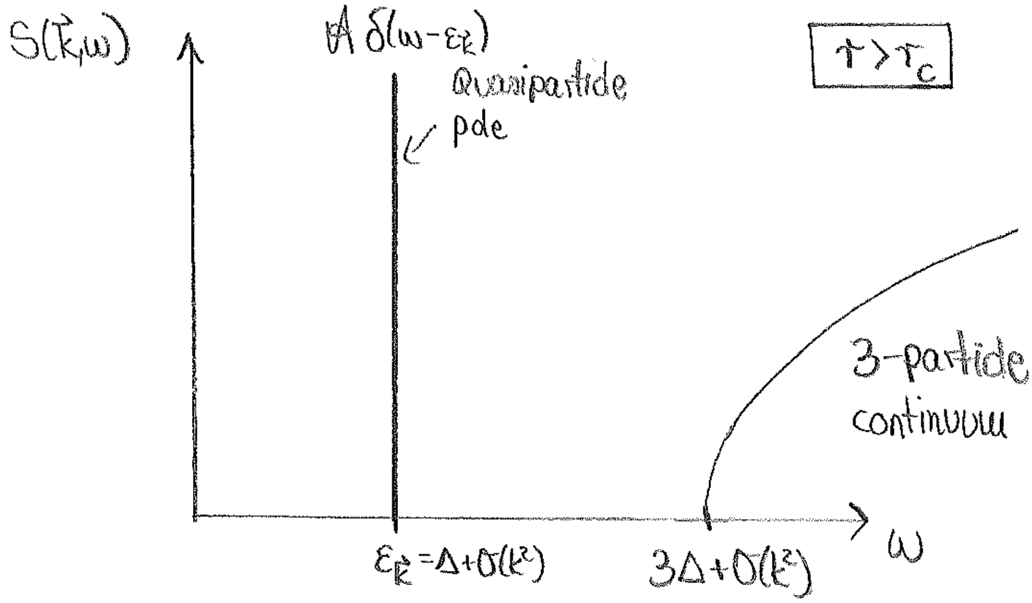
from $\frac{u}{4!}\phi^4$ selfinteraction

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

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

Remarks:

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



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Limit $r \searrow r_c$:

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

$\Rightarrow$ scaling of single-particle pole: $\mathcal{A} \propto \Delta^{\eta} \propto (r-r_c)^{\eta\nu} \quad (z=1)$

Ordered phase $(r<r_c)$:

$$S(\vec{k},\omega) = N_0^2\, (2\pi)^{d+1}\, \delta(\omega)\,\delta(\vec{k}) + \mathcal{O}(\omega)$$

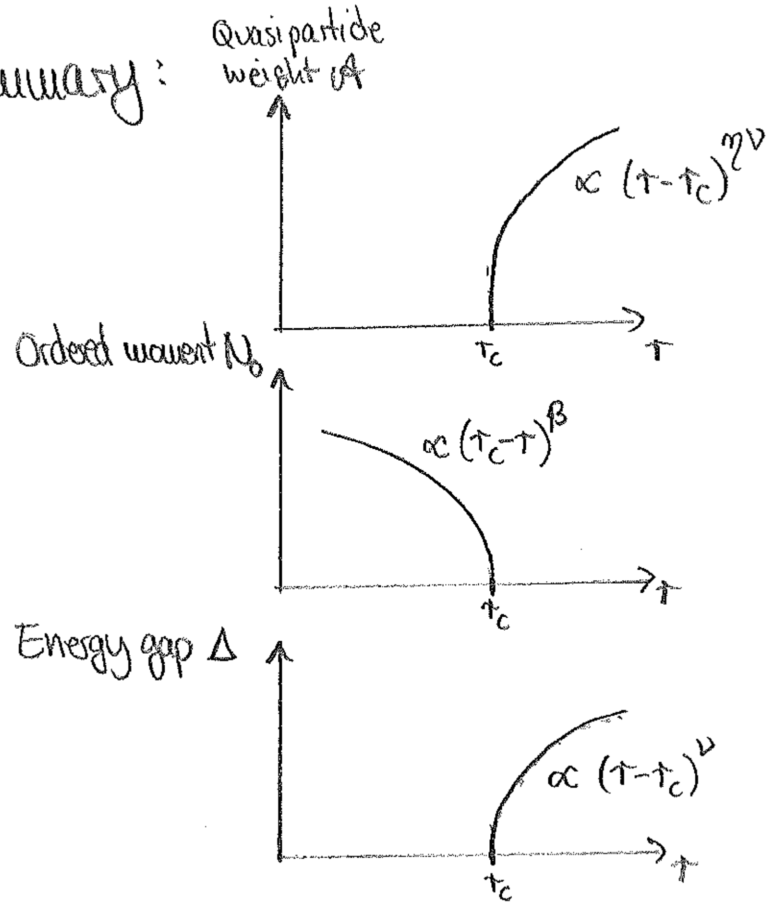
N_0: order parameter

"Bragg peak at $\vec{k}=0$"

Susceptibility $(N>1)$:

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

Summary:



7.3 Quantum Ising chain

Hamiltonian:

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

Strong-coupling limit $g \gg 1$

Ground state:

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

  "polarized state"

- $g < \infty$: $\quad |\Psi_0\rangle = \prod_i |\rightarrow\rangle_i - \frac{1}{2g} \sum_i |\rightarrow_1 \cdots \rightarrow_{i-1} \leftarrow_i \leftarrow_{i+1} \rightarrow_{i+2} \cdots \rightarrow_M\rangle$

  $+\mathcal{O}\left(\frac{1}{g^2}\right)$

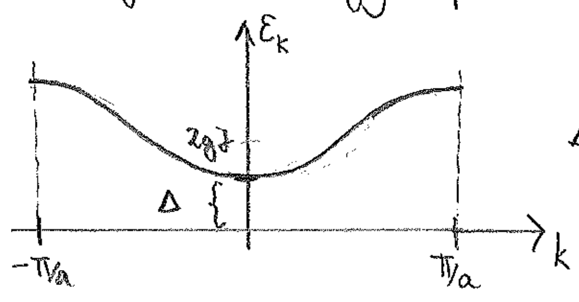
  since $\sigma_i^z |\rightarrow\rangle_i = |\leftarrow\rangle_i$ "spin-flip operator"

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

One-particle excitations:

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

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



$$\Delta = 2J(g-1) + \mathcal{O}\left(\tfrac{1}{g}\right)$$

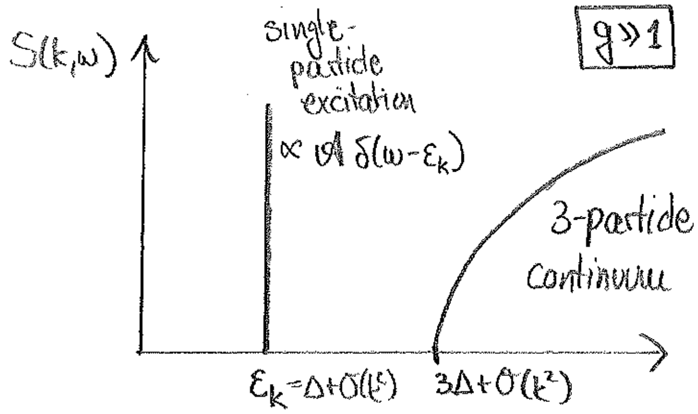
Two-particle excitations:

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



Weak-coupling limit $g \ll 1$

Correlation function:

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

Ground state:

- $g=0$:

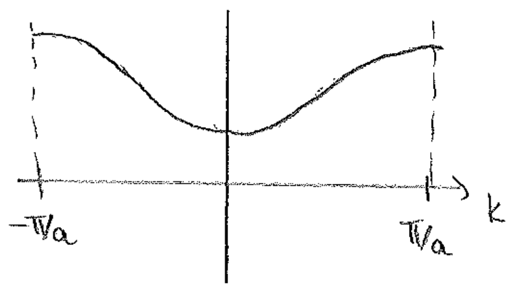
$$|\Psi_0\rangle = \begin{cases} \prod_i |\uparrow\rangle_i \\ \prod_i |\downarrow\rangle_i \end{cases}$$

- $g>0$:

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

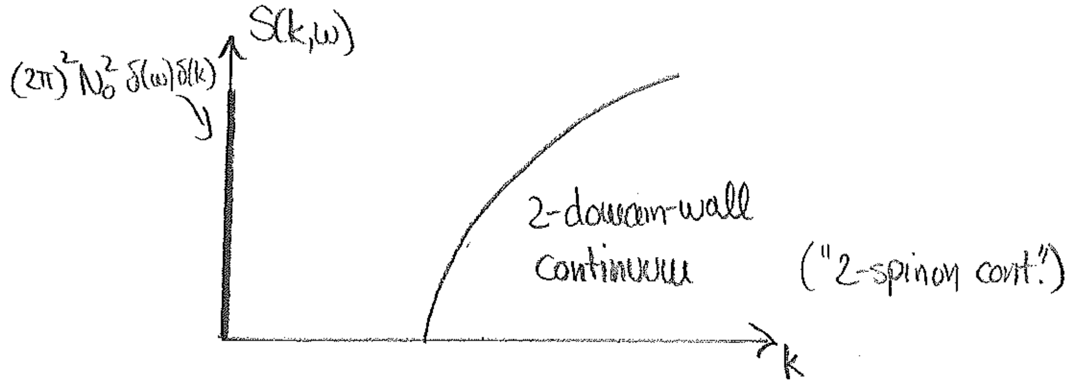
One-particle excitations:

- $g=0$: $|i\rangle = |\ldots\uparrow\downarrow_i\downarrow\downarrow\ldots\rangle$ with $\varepsilon = 2J$ (domain wall at i)
- $g>0$: $|k\rangle = \frac{1}{\sqrt{N}}\sum_i e^{ikx_i}|i\rangle$ with $\varepsilon_k = J(2-2g\cos ka) + \mathcal{O}(g^2)$



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:

$$\sigma_i^z = 1 - 2\, c_i^\dagger c_i$$

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

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

with $\sigma_i^\pm = \sigma_i^x \pm i \sigma_i^y$ and

$$\{c_i, c_j^\dagger\} = \delta_{ij} \qquad \text{fermions}$$

Inverse transformation:

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

$$c_i^\dagger = \Big(\prod_{j<i} \sigma_j^z \Big) \sigma_i^-$$

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

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

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

Fourier transformation :

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

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 $\gamma_k, \gamma_k^\dagger$:

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

with dispersion:

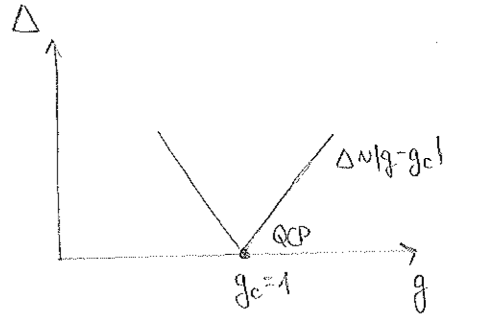
$$\varepsilon_k = 2J\sqrt{1 + g^2 - 2g\cos ka} \geq 0$$

Band gap:

$$\Delta = \varepsilon_{k=0} = 2J\,|1-g| = 0 \iff g = g_c = 1$$

Critical behavior

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



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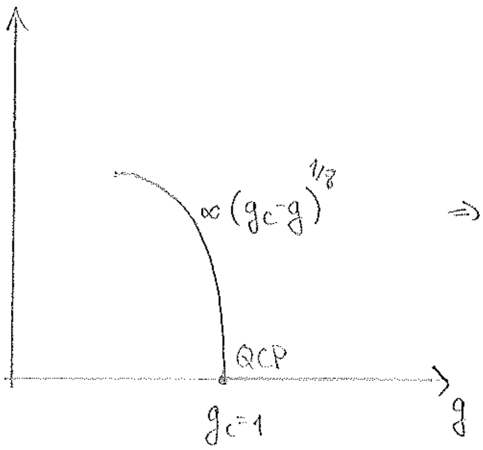
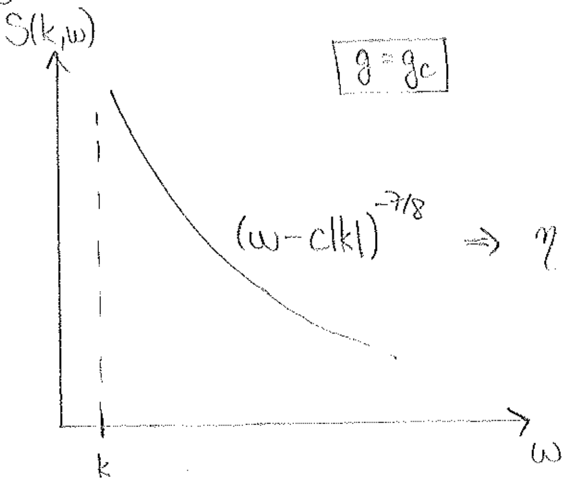
Further results (from exact solution):

Order parameter: N_0

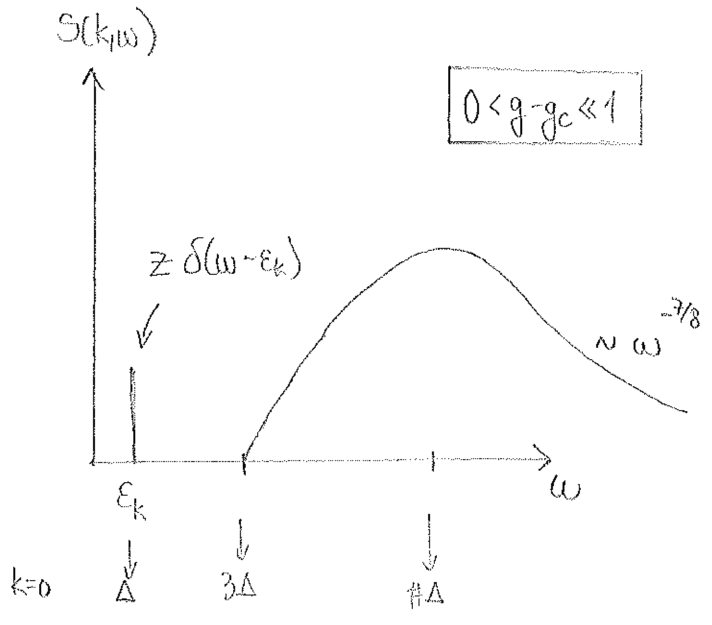


$\Rightarrow \beta = 1/8$

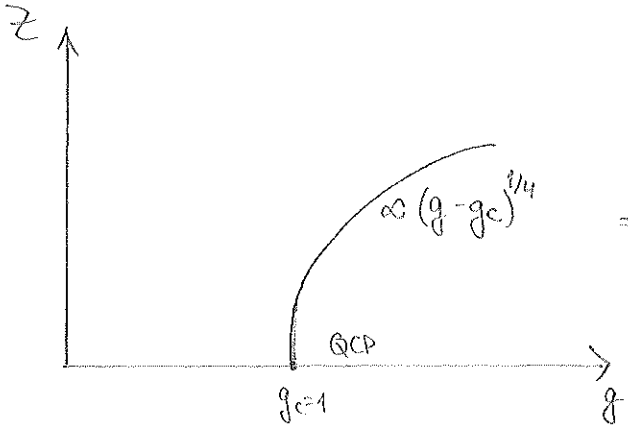
Dynamic structure factor:



$\Rightarrow \eta = \frac{1}{4}$

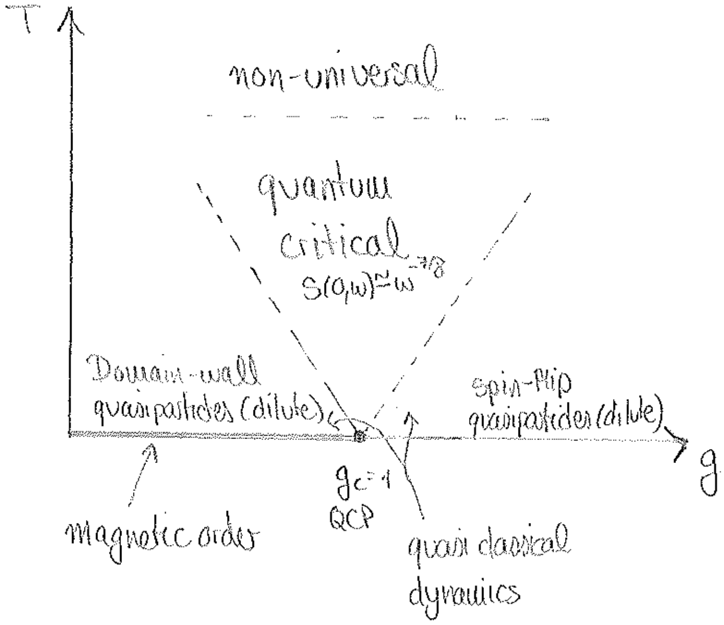


Flipped-spin quasiparticle weight ($g > g_c$):



$\Rightarrow \quad \eta\nu = \frac{1}{4}$

Finite-temperature phase diagram:



Critical exponents:

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

$$z = 1$$