Linear response

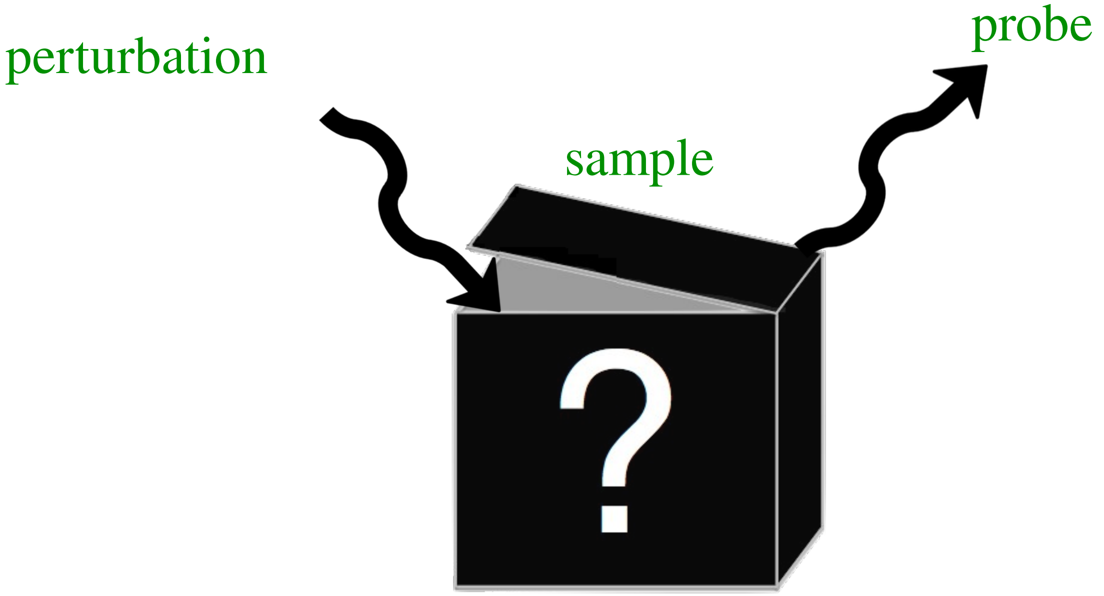
Kubo formula

$$\langle A(t)\rangle_\phi - \langle A\rangle_0 = i\int_{-\infty}^{t} dt' \langle [\tilde{B}(t'), \tilde{A}(t)]\rangle_0 \phi(t') = i\int_{-\infty}^{\infty} dt' \Theta(t-t')\langle [\tilde{B}(t'), \tilde{A}(t)]\rangle_0 \phi(t')$$
$$\equiv \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t')\phi(t')$$

Response of a system to small external perturbations is described by ground state (equilibrium)
correlation functions (fluctuation-dissipation theorem).

$\langle c^\dagger(t) c(t')\rangle$	photoemission
$\langle \vec{j}(t)\vec{j}(t')\rangle$	conductivity, optical absorption
$\langle \vec{S}(t)\vec{S}(t')\rangle$	magnetic susceptibility
$\langle c_\uparrow^\dagger(t) c_\downarrow^\dagger(t) c_\downarrow(t') c_\uparrow(t')\rangle$	superconductivity

$\vec{S}, \vec{j} \sim c^\dagger c$ (semi-local) density-like quantities



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$$\equiv \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t')\phi(t')$$

Response of a system to small external perturbations is described by ground state (equi… corre…).

spin: $a_\downarrow^\dagger a_\uparrow + a_\uparrow^\dagger a_\downarrow$, $i(a_\downarrow^\dagger a_\uparrow - a_\uparrow^\dagger a_\downarrow)$, $a_\uparrow^\dagger a_\uparrow - a_\downarrow^\dagger a_\downarrow$ $\;\Rightarrow\;$ $\boldsymbol{\sigma}_{\alpha\beta} a_\alpha^\dagger a_\beta$

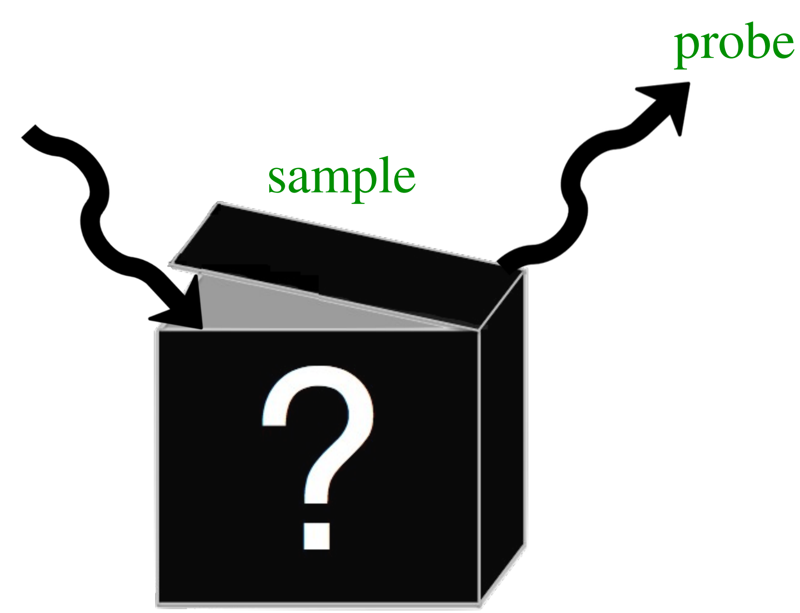
charge: $a_\uparrow^\dagger a_\uparrow + a_\downarrow^\dagger a_\downarrow$ $\;\Rightarrow\;$ $\sigma^0_{\alpha\beta} a_\alpha^\dagger a_\beta$

$\langle c^\dagger$

$\langle \vec{j}$

$\langle \vec{S}$

$\langle c_\uparrow^\dagger(t) c_\downarrow^\dagger($ … superconductivity



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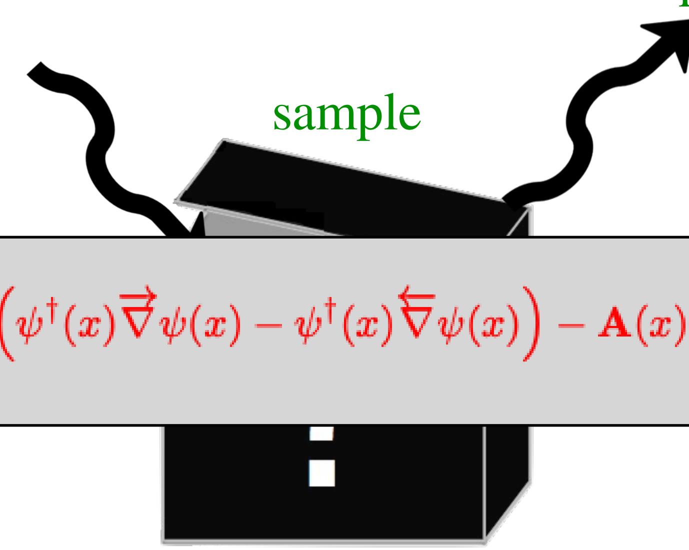

$\langle c^\dagger(t)c(t')\rangle$ photoemission

$\langle \vec{j}(t)\vec{j}(t')\rangle$ conductivity, optical absorption

$\langle \vec{S}$

$\langle c^\dagger_\uparrow(t)c^\dagger_\downarrow(t$ superconductivity

charge current $it(a^\dagger_{i,\alpha}a_{i+1,\alpha} - a^\dagger_{i+1,\alpha}a_{i,\alpha})$ $-\frac{i}{2}\left(\psi^\dagger(x)\overrightarrow{\nabla}\psi(x) - \psi^\dagger(x)\overleftarrow{\nabla}\psi(x)\right) - \mathbf{A}(x)\psi^\dagger(x)\psi(x)$

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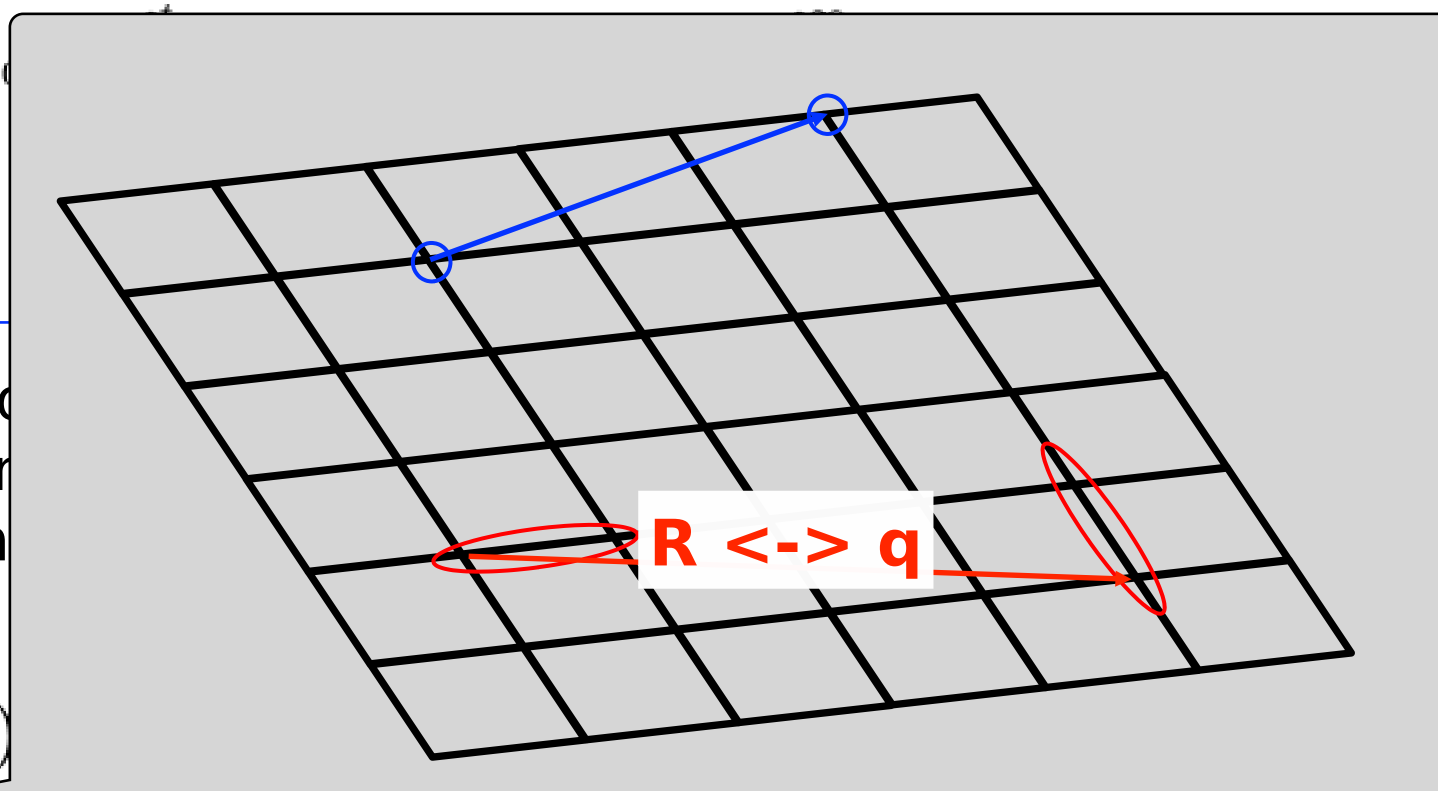
Linear response

Kubo formula

$\langle A(t)\rangle_\phi - \langle A\rangle_{\ldots}$ ... $t')$



Response ... cribed by ground state
(equilibriu...
correlation...

$\langle c^\dagger(t)c(t')$ ...

$\langle \vec{j}(t)\,\vec{j}(t')\rangle$ conductivity, optical absorption

$\langle \vec{S}(t)\,\vec{S}(t')\rangle$ magnetic susceptibility

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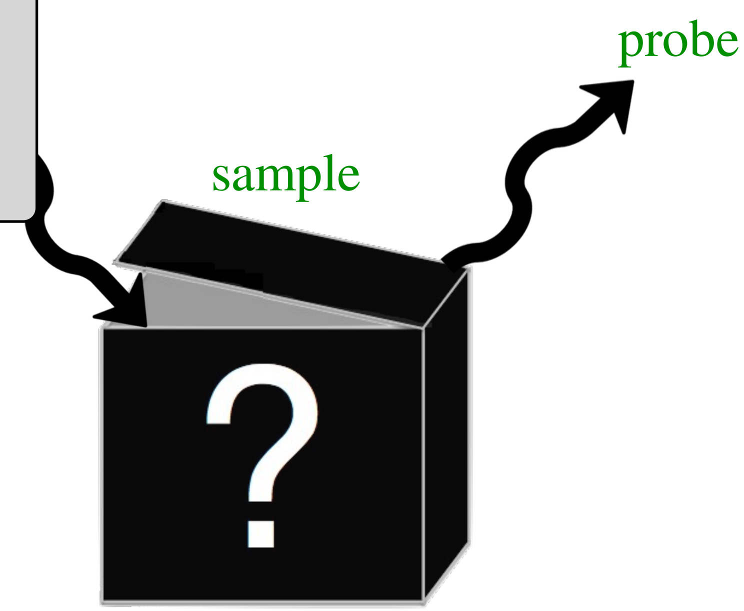
$\vec{S},\,\vec{j} \sim c^\dagger c$ (semi-local) density-like quantities

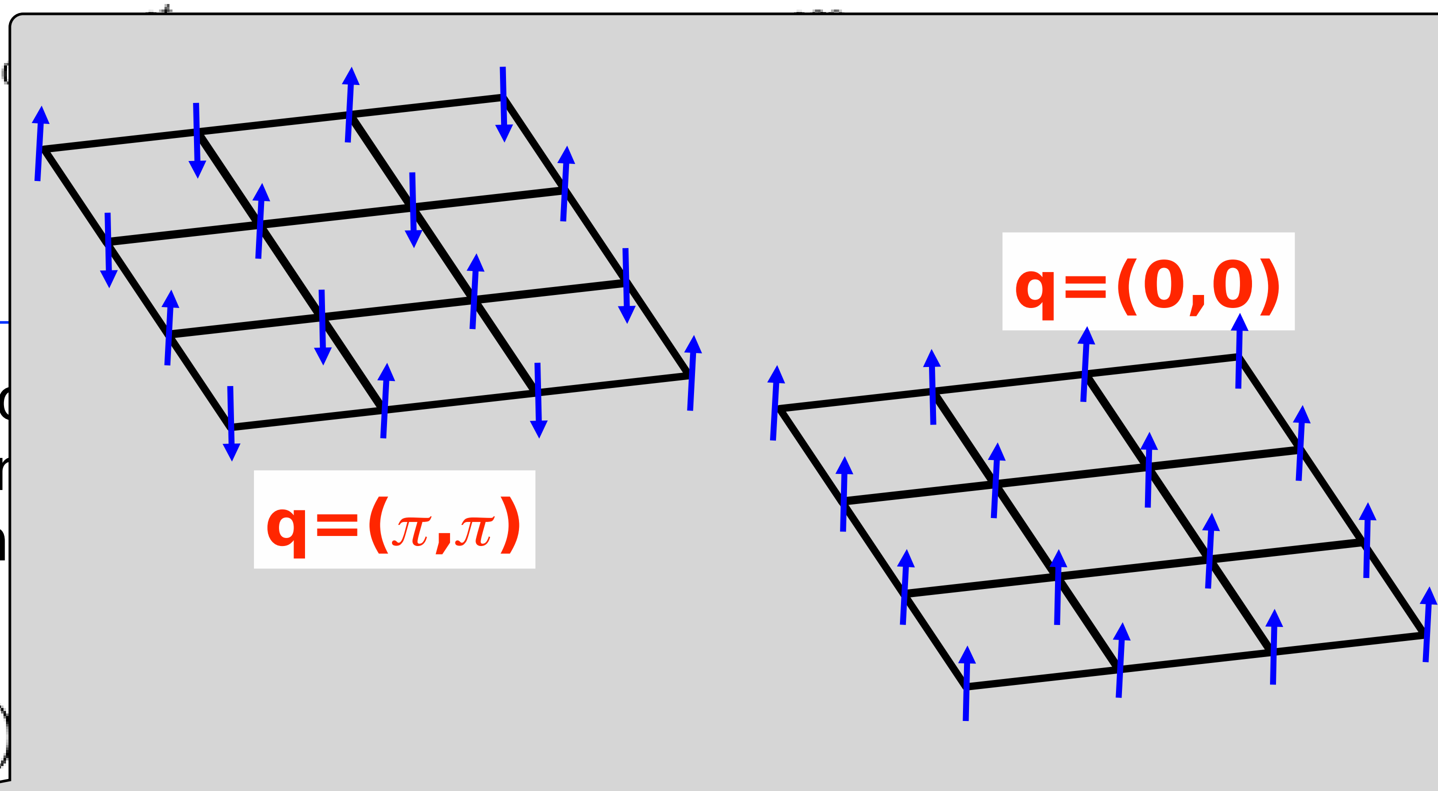


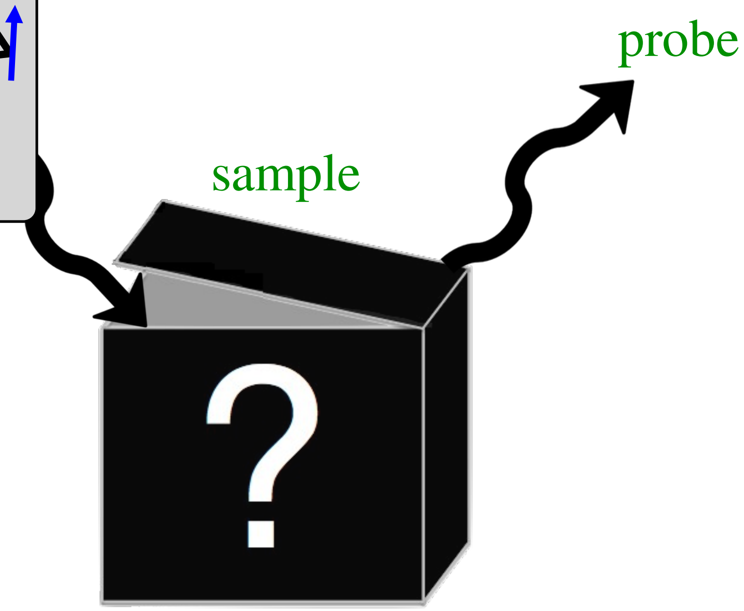
Linear response

Kubo formula

$\langle A(t)\rangle_\phi - \langle A\rangle_($ … $t')$

Response c… cribed by ground state
(equilibriu…
correlation…





$\langle c^\dagger(t)c(t')$ …

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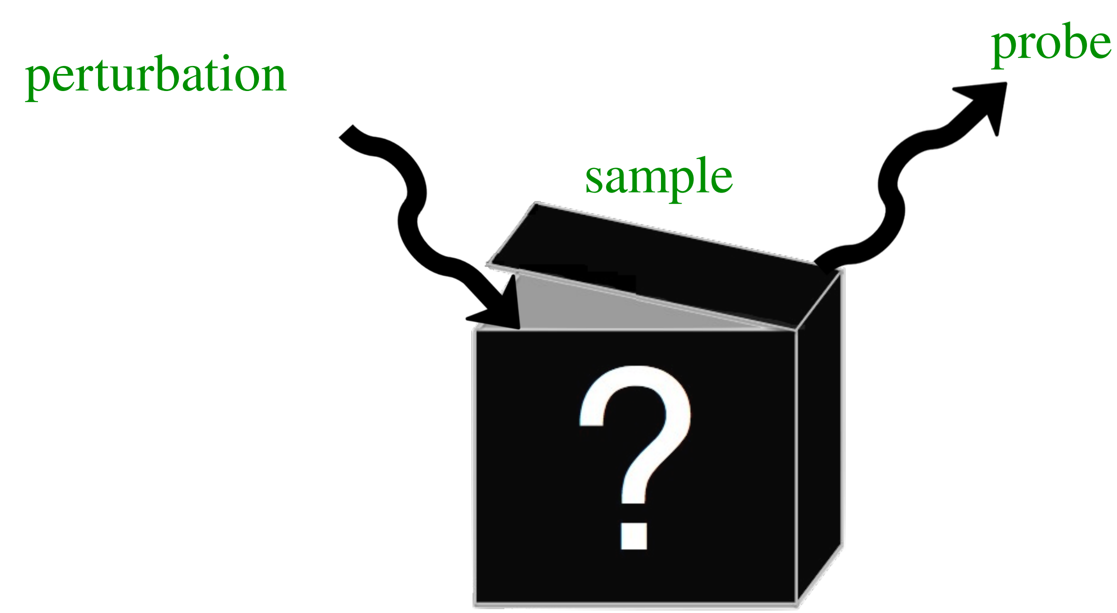

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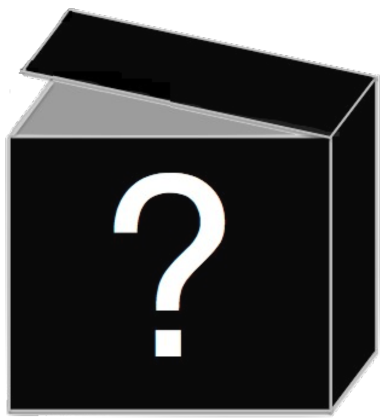
Let us consider the response to static perturbations $\phi(t) = \phi, \quad \phi(\omega) = \phi\delta_{\omega 0}$

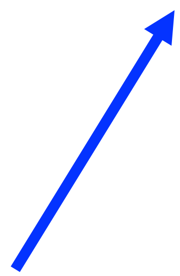
Susceptibility

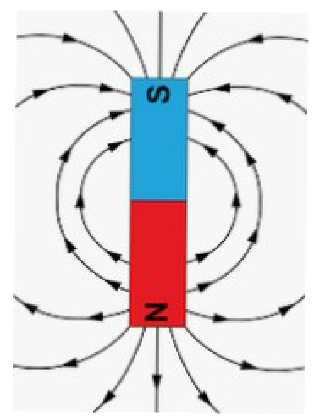
$$\langle A(t)\rangle_\phi - \langle A\rangle_0 = \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t')\phi(t')$$

Thermodynamic definition of susceptibility

$$\hat{H} \quad - \quad \hat{\mathbf{M}} \cdot \mathbf{h}$$







@T=0

$$M_\alpha \equiv \langle \psi_g | \hat{M}_\alpha | \psi_g \rangle = -\frac{\delta E_g}{\delta h_\alpha}$$

=0 (by minimum property of the ground state)

$$-\frac{\delta}{\delta h_\alpha}\langle \psi_g | \hat{H}(\mathbf{h}) | \psi_g \rangle = -\langle \frac{\delta \psi_g}{\delta h_\alpha} | \hat{H}(\mathbf{h}) | \psi_g \rangle - \langle \psi_g | \hat{H}(\mathbf{h}) | \frac{\delta \psi_g}{\delta h_\alpha} \rangle$$

$$- \langle \psi_g | \frac{\delta \hat{H}(\mathbf{h})}{\delta h_\alpha} | \psi_g \rangle$$

$$= \langle \psi_g | M_\alpha | \psi_g \rangle$$

@T>0

$$M_\alpha = -\frac{\delta F}{\delta h_\alpha}$$ <- free energy

$$\boxed{\chi_{\alpha\beta} = \left.\frac{\delta M_\alpha}{\delta h_\alpha}\right|_{h=0} = -\left.\frac{\delta^2 F}{\delta h_\alpha \delta h_\beta}\right|_{h=0}}$$

Susceptibility

$$\langle A(t)\rangle_\phi - \langle A\rangle_0 = \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t')\phi(t')$$

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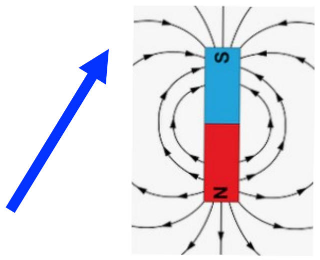
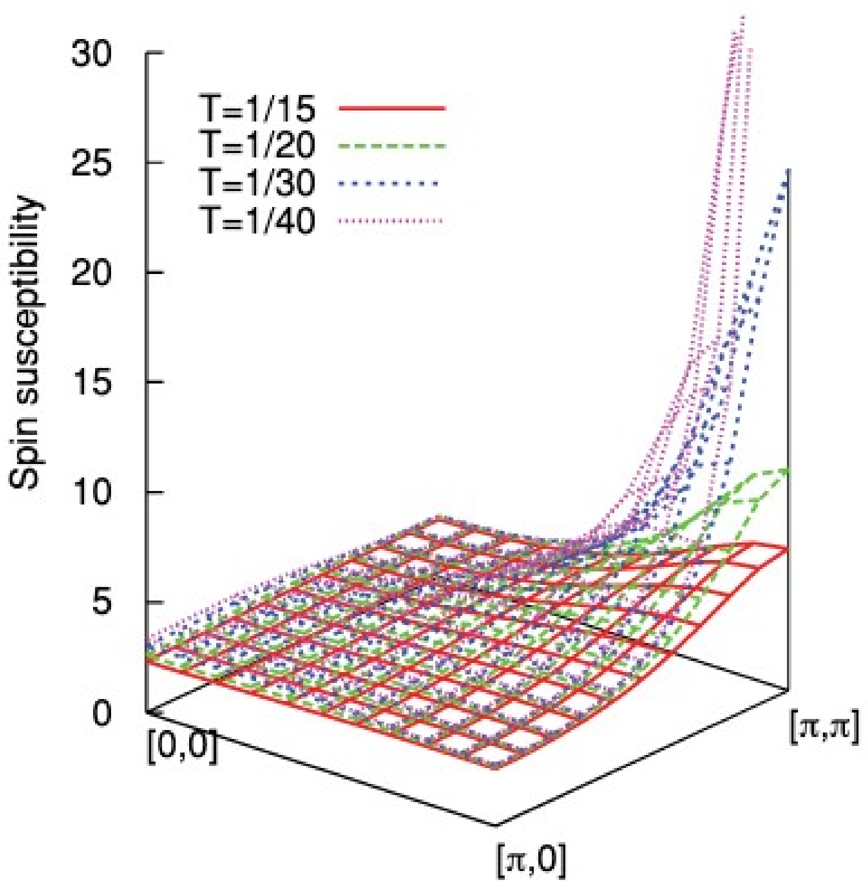
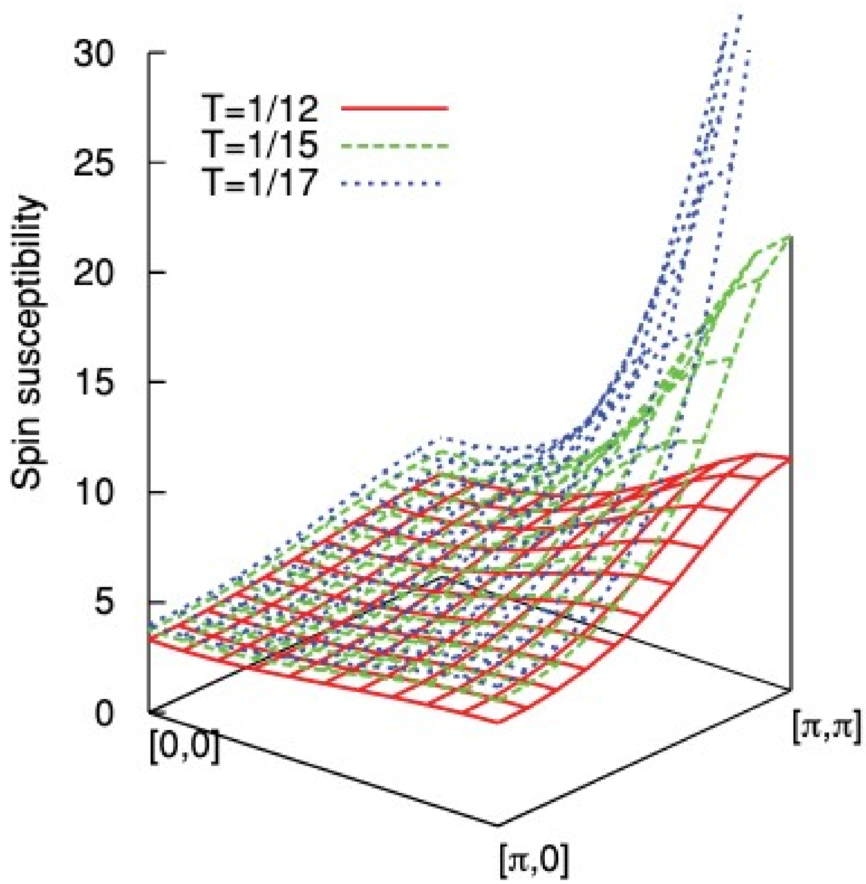


What if the susceptibility diverges?

2D Hubbard model (DMFT solution)



U=0.4



U=1

Susceptibility

$$\langle A(t)\rangle_\phi - \langle A\rangle_0 = \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t')\phi(t')$$

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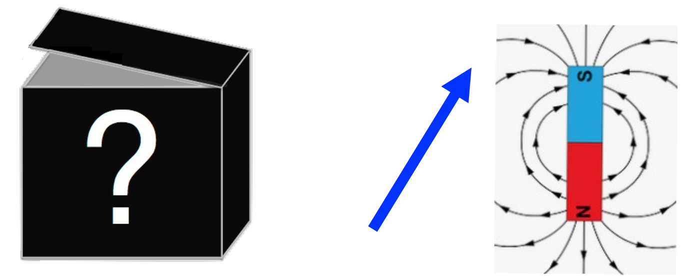

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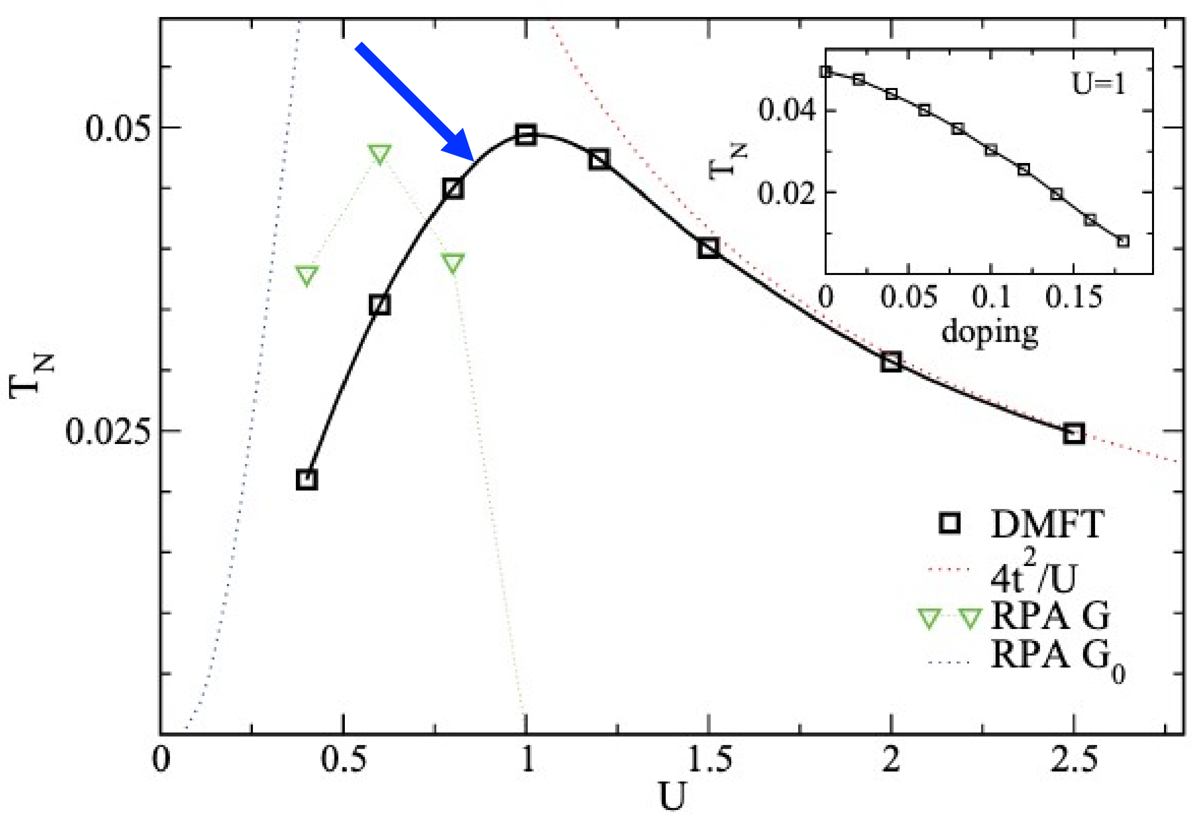
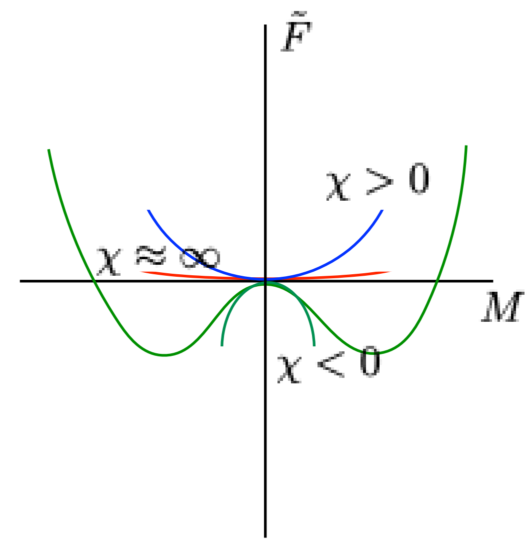


$$\tilde{F}(M) = \min_h\{F(h) + hM\} \qquad M = -\frac{\delta F}{\delta h}$$

$$\frac{\delta \tilde{F}}{\delta M} = \frac{\delta F}{\delta h}\frac{\delta h}{\delta M} + M\frac{\delta h}{\delta M} + h = h$$

$$\frac{\delta^2 \tilde{F}}{\delta M^2} = \frac{\delta h}{\delta M} = \chi^{-1}$$



Susceptibility

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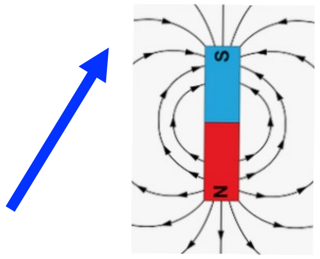

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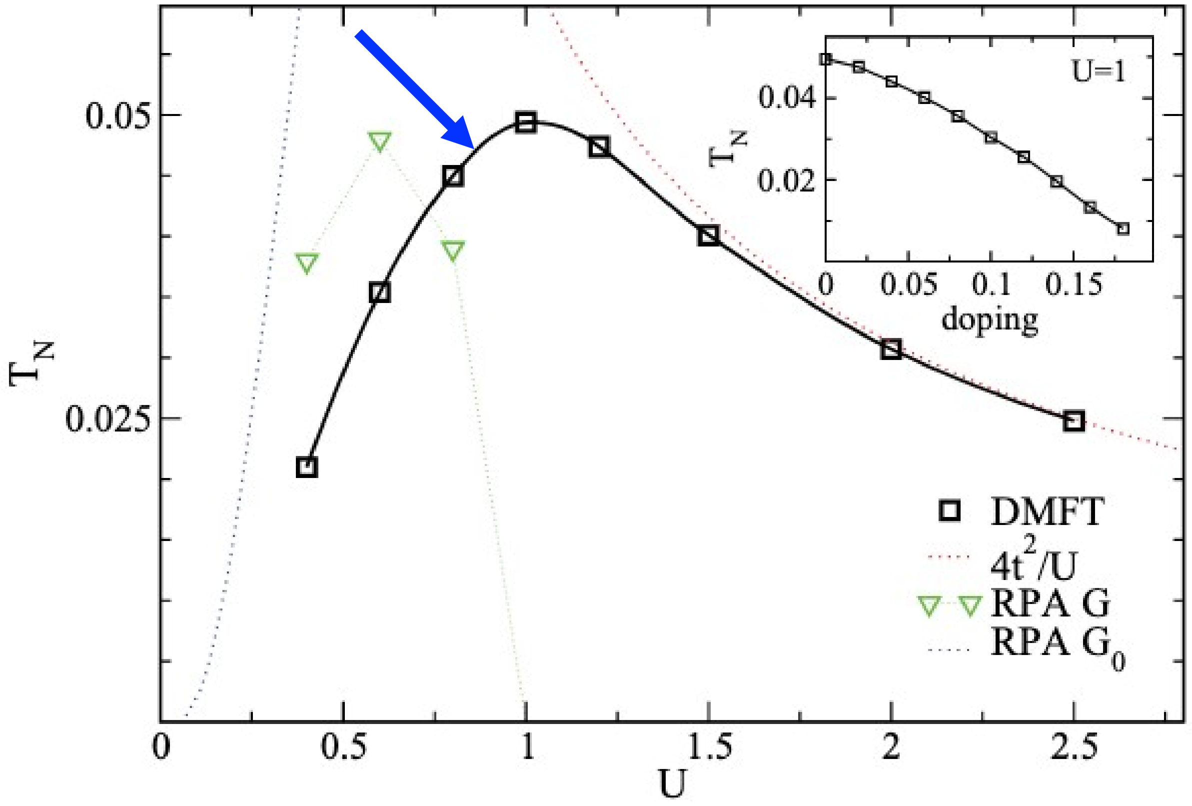

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$$\frac{\delta \tilde{F}}{\delta M} = \frac{\delta F}{\delta h}\frac{\delta h}{\delta M} + M\frac{\delta h}{\delta M} + h = h$$

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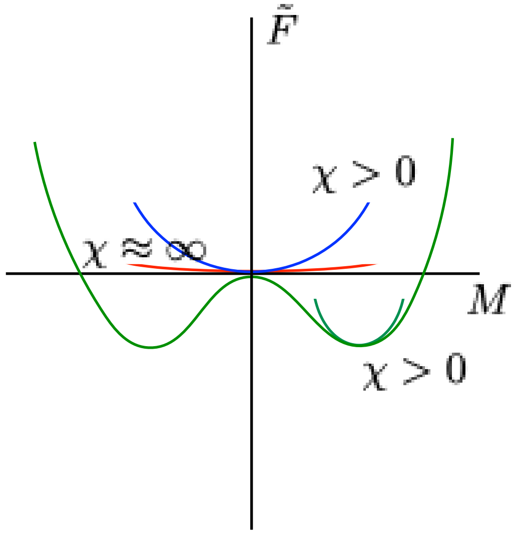
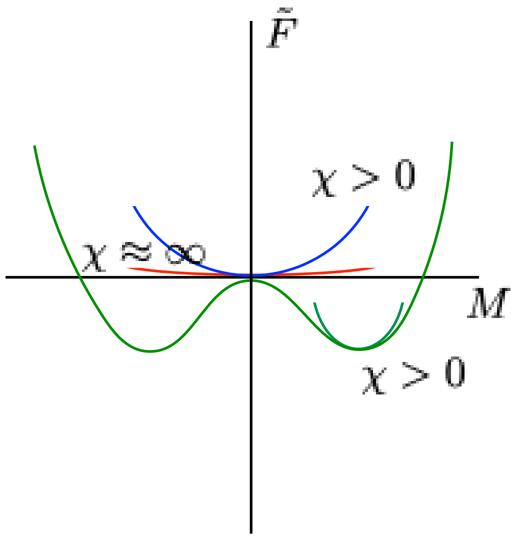


Critical phenomena

How does susceptibility and other quantities (e.g. M) as a function of control parameter (e.g. temperature) approach the critical point?



$$M \sim \left(1 - \frac{T}{T_c}\right)^{\beta}$$

$$\chi \sim \left(\frac{T}{T_c} - 1\right)^{-\gamma}$$

Example: Ising model

	d=2	d=3	d=4
β	1/8	0.326419(3)	1/2
γ	7/4	1.237075(10)	1

Dimension is crucial!

Correlation length

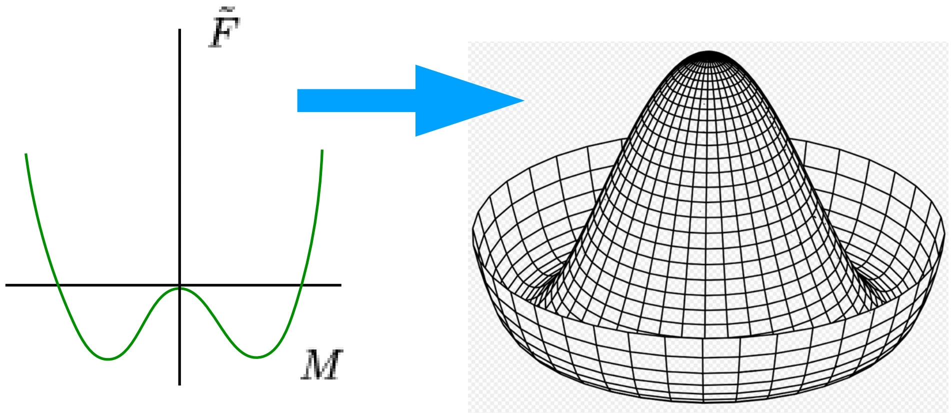
The static susceptibility "collects" temporal correlations over all time-scales.

Can we detect a symmetry breaking "instantaneously"? Yes

In the normal state $\langle M_i M_j \rangle \sim \exp(-\frac{|R_i - R_j|}{\lambda})$ for large distances.

When the transition is approached the correlation length λ diverges, i.e., the correlation function
does not diverges exponentially at the transition.

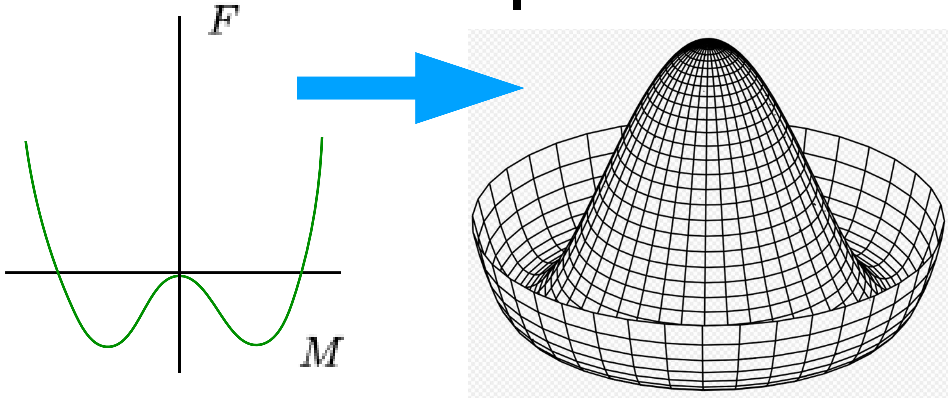
Spontaneous breaking of continuous symmetry



Continuous symmetries: space isotropy (orbital or spin rotations),
space homogeneity (translation), gauge symmetries (charge conservation)

Transition:	**Broken symmetry**
liquid, gas -> solid	translation (homogeneity of space)
paramagnet -> ferromagnet	spin rotation (isotropy of spin space)
paramagnet-> antiferromagnet	spin rotation (isotropy of spin space)
metal -> superconductor	gauge symmetry (charge conservation)
normal gas -> Bose-Einstein condensate	gauge symmetry (particle number conservation)

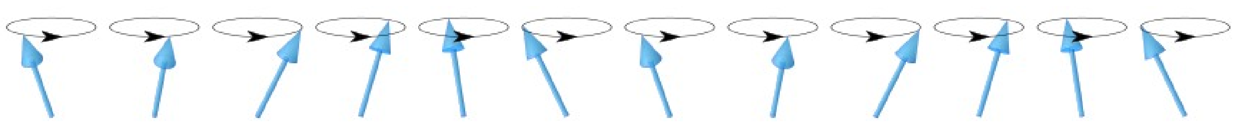
Spontaneous breaking of continuous symmetry

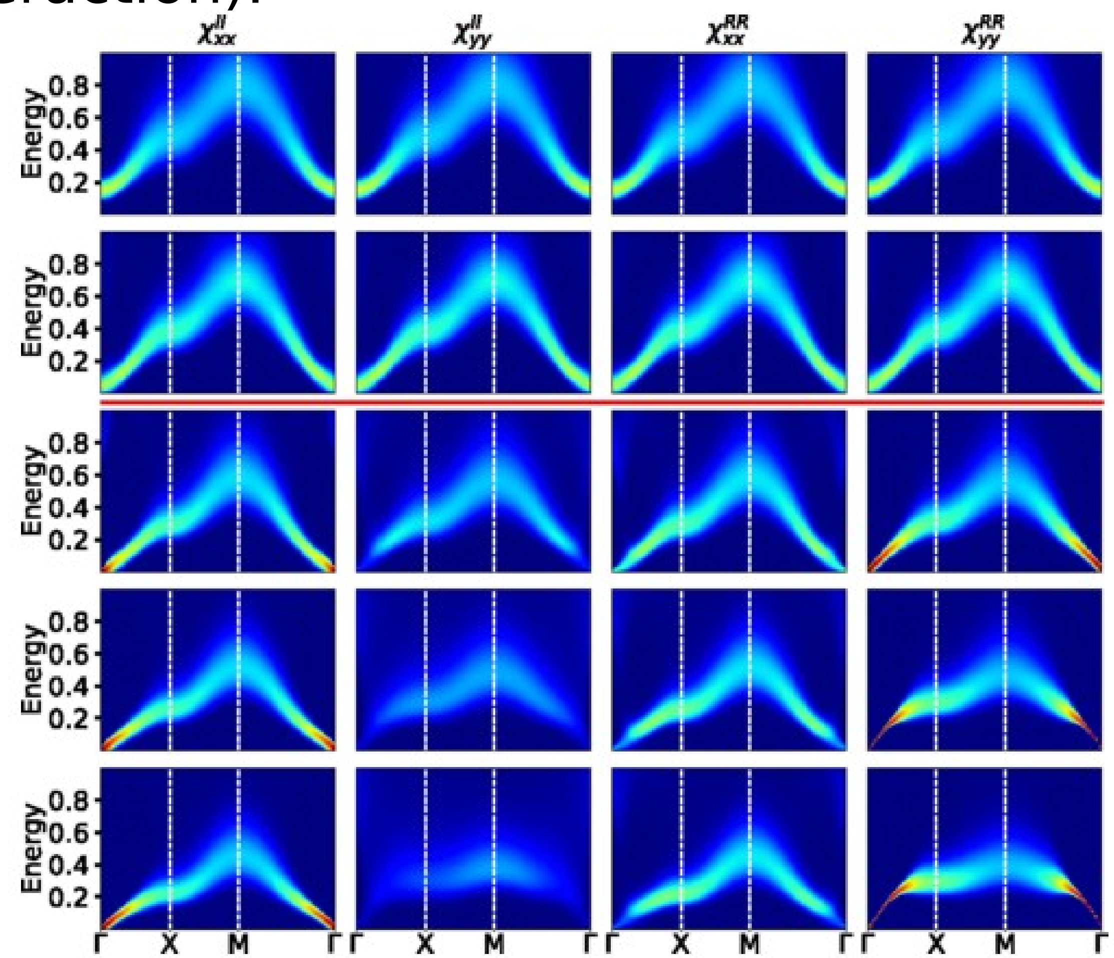


Continuous symmetries: space isotropy (orbital or spin rotations),
space isotropy (translation), gauge symmetries (charge conservation)

Goldstone mode (in systems with short-range interaction):

Long-wave length rotations of the order parameter cost vanishingly low energy.





2 linear modes in 2-orbital Hubbard model (exciton condensate phase)

Transition:

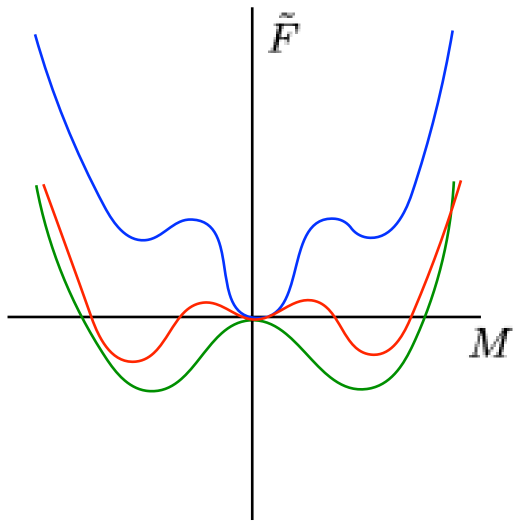
liquid, gas -> solid
paramagnet -> ferromagnet
paramagnet-> antiferromagnet
metal -> superconductor
normal gas -> Bose-Einstein condensate

Goldstone mode

acoustic phonons
(quadratic) magnons
(linear) magnons
massive (due to long-range Coulomb interaction)
'sound' waves

Not all transitions are associated with divergent susceptibility

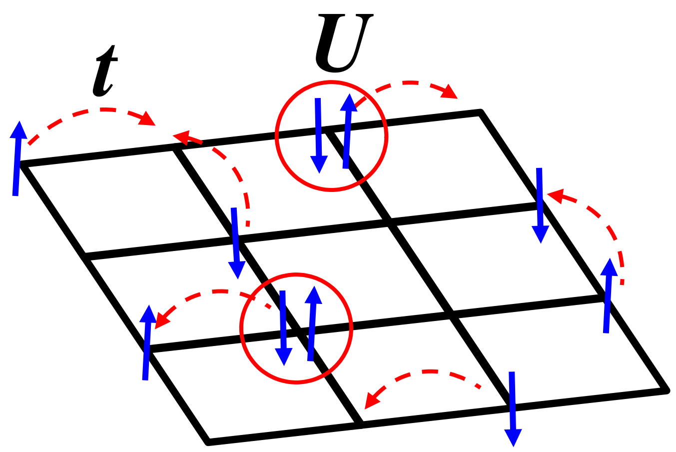
First order transitions (distinct states are locally stable,
while their energies cross):
The transition does not have to break any symmetry
(e.g. vapor <-> liquid transition)



Topological transitions (no local order parameter), the phases are distinguished by (discrete) topological invariants

Spontaneous symmetry breaking (mean-field theory)

Hubbard model (simplest model that have all the ingredients) at half filling n=1



$$H = -\mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma} + t \sum_{ij,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

$$c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \equiv n_{i\uparrow} n_{i\downarrow} = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) - \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})^2$$

$$H = H_0 - \frac{U}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})^2 \equiv H_0 - \frac{U}{2} \sum_i m_{iz}^2$$

Mean-field decoupling (T=0)

$$H = H_{\rm MF} + \Delta H \qquad H_{\rm MF} = H_0 - U \sum_i M_i m_{iz} \qquad \Delta H = -\frac{U}{2} \sum_i m_{iz}^2 + U \sum_i M_i m_{iz}$$

$$\langle H \rangle \leq \langle H \rangle_{\rm MF} = \langle H_{\rm MF} + \Delta H \rangle_{\rm MF} = \langle H_{\rm MF} \rangle_{\rm MF} + \langle \Delta H \rangle_{\rm MF}$$

$$\langle \Delta H \rangle_{\rm MF} = \frac{U}{2} \left(2 \sum_i M_i \langle m_{iz} \rangle_{\rm MF} - \sum_i \langle m_{iz} \rangle^2_{\rm MF} \right)$$

Minimize $\quad \frac{\partial}{\partial M_i} \langle H \rangle_{\rm MF} = 0$

$$\frac{\partial}{\partial M_i} \langle H_{\rm MF} \rangle_{\rm MF} = \langle \frac{\partial H_{\rm MF}}{\partial M_i} \rangle_{\rm MF} = -U \langle m_{iz} \rangle_{\rm MF}$$

$$\frac{\partial}{\partial M_i} \langle \Delta H \rangle_{\rm MF} = U \langle m_{iz} \rangle_{\rm MF} + U M_i \frac{\partial}{\partial M_i} \langle m_{iz} \rangle_{\rm MF} - U \langle m_{iz} \rangle_{\rm MF} \frac{\partial}{\partial M_i} \langle m_{iz} \rangle_{\rm MF}$$

$$\Longrightarrow \; M_i = \langle m_{iz} \rangle_{\rm MF} \qquad \Longrightarrow \; \langle H \rangle_{\rm MF} = \langle H_{\rm MF} \rangle_{\rm MF} + \frac{U}{2} \sum_i M_i^2$$

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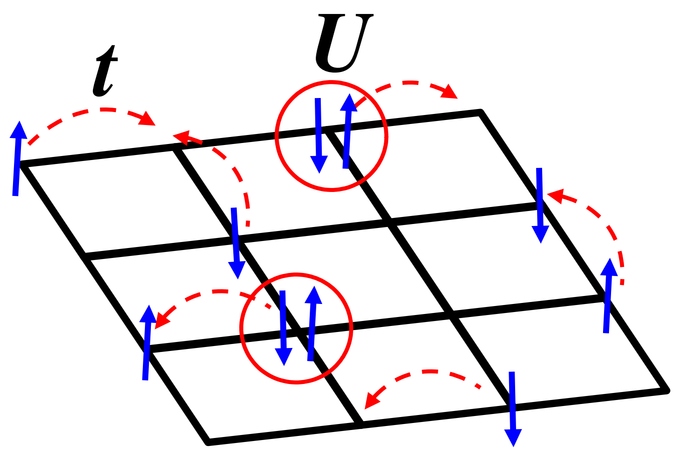

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$$H = H_0 - \frac{U}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})^2 \equiv H_0 - \frac{U}{2} \sum_i m_{iz}^2$$

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$$\langle H \rangle \leq \langle H \rangle_{\mathrm{MF}} = \langle H_{\mathrm{MF}} + \Delta H \rangle_{\mathrm{MF}} = \langle H_{\mathrm{MF}} \rangle_{\mathrm{MF}} + \langle \Delta H \rangle_{\mathrm{MF}}$$

$$\langle \Delta H \rangle_{\mathrm{MF}} = \frac{U}{2} \left(2 \sum_i M_i \langle m_{iz} \rangle_{\mathrm{MF}} - \sum_i \langle m_{iz} \rangle^2_{\mathrm{MF}} \right)$$

Minimize $\frac{\partial}{\partial M_i} \langle H \rangle_{\mathrm{MF}} = 0$

$$\frac{\partial}{\partial M_i} \langle H_{\mathrm{MF}} \rangle_{\mathrm{MF}} = \langle \frac{\partial H_{\mathrm{MF}}}{\partial M_i} \rangle_{\mathrm{MF}} = -U \langle m_{iz} \rangle_{\mathrm{MF}}$$

$$\frac{\partial}{\partial M_i} \langle \Delta H \rangle_{\mathrm{MF}} = U \langle m_{iz} \rangle_{\mathrm{MF}} + U M_i \frac{\partial}{\partial M_i} \langle m_{iz} \rangle_{\mathrm{MF}} - U \langle m_{iz} \rangle_{\mathrm{MF}} \frac{\partial}{\partial M_i} \langle m_{iz} \rangle_{\mathrm{MF}}$$

$$\Longrightarrow \boxed{M_i = \langle m_{iz} \rangle_{\mathrm{MF}}} \qquad \Longrightarrow \boxed{\langle H \rangle_{\mathrm{MF}} = \langle H_{\mathrm{MF}} \rangle_{\mathrm{MF}} + \frac{U}{2} \sum_i M_i^2}$$

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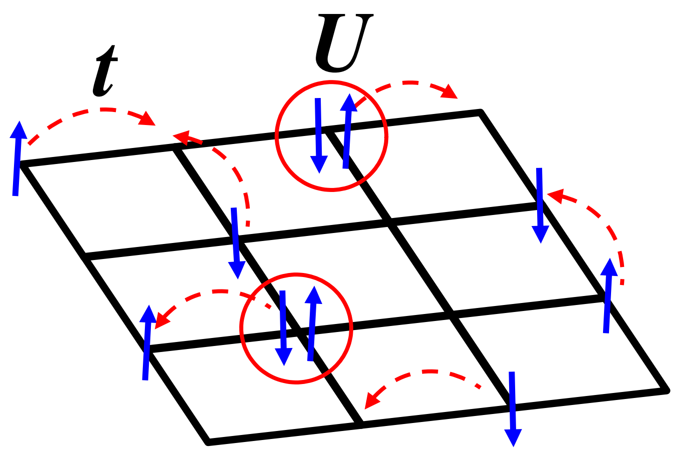


$$H = -\mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma} + t \sum_{ij,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

$$c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} \equiv n_{i\uparrow} n_{i\downarrow} = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) - \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})^2$$

$$H = H_0 - \frac{U}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})^2 \equiv H_0 - \frac{U}{2} \sum_i m_{iz}^2$$

Mean-field decoupling (T=0)

Intuitive picture:

Write the operator a expectation value plus 'fluctuations'

$$m_{iz} = M_i + (m_{iz} - M_i)$$

Keep only linear terms in the 'fluctuations'

$$m_{iz}^2 \approx M_i^2 + 2M_i(m_{iz} - M_i) = 2M_i m_{iz} - M_i^2$$

$$\frac{\partial}{\partial M_i} \langle \Delta H \rangle_{\mathrm{MF}} = U \langle m_{iz} \rangle_{\mathrm{MF}} + U M_i \frac{\partial}{\partial M_i} \langle m_{iz} \rangle_{\mathrm{MF}} - U \langle m_{iz} \rangle_{\mathrm{MF}} \frac{\partial}{\partial M_i} \langle m_{iz} \rangle_{\mathrm{MF}}$$

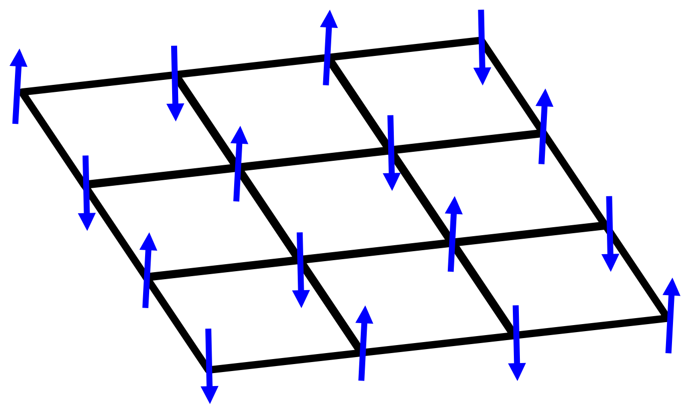
$$\Longrightarrow \boxed{M_i = \langle m_{iz} \rangle_{\mathrm{MF}}} \qquad \Longrightarrow \boxed{\langle H \rangle_{\mathrm{MF}} = \langle H_{\mathrm{MF}} \rangle_{\mathrm{MF}} + \frac{U}{2} \sum_i M_i^2}$$

Spontaneous symmetry breaking (mean-field theory)

Hubbard model (simplest model that have all the ingredients)

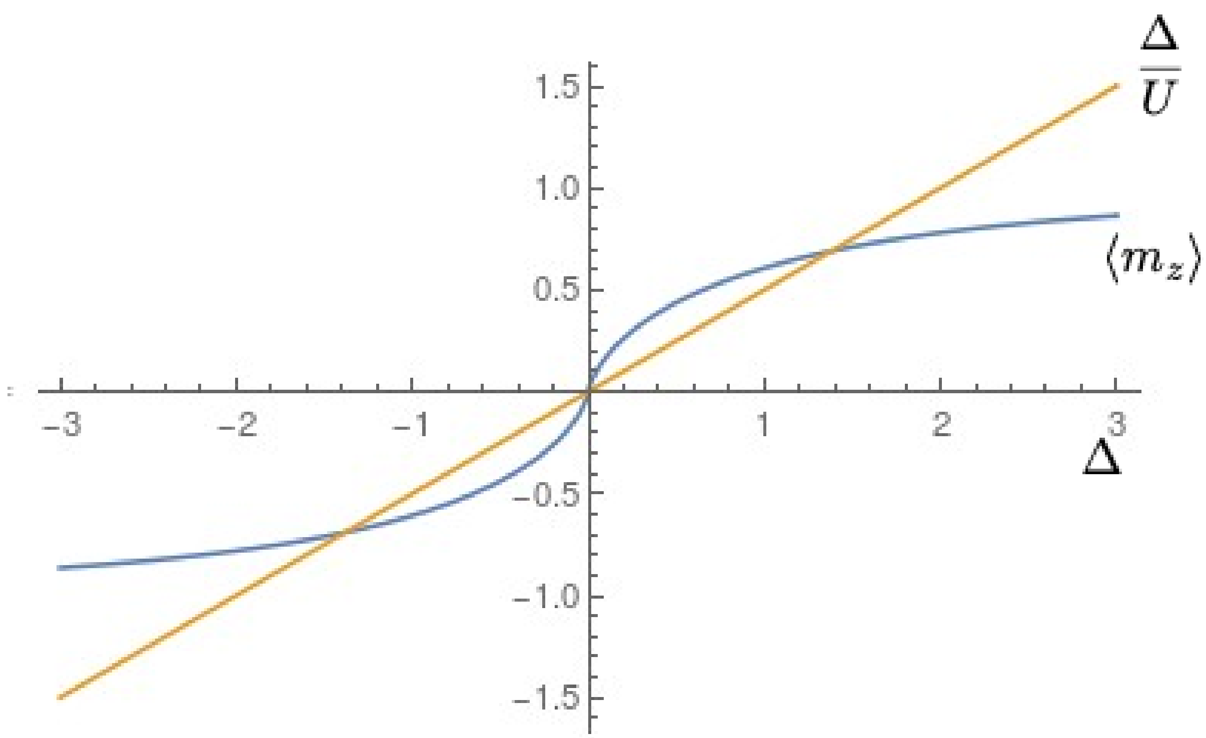
Assuming staggered order:
$M_i = (-1)^i M$

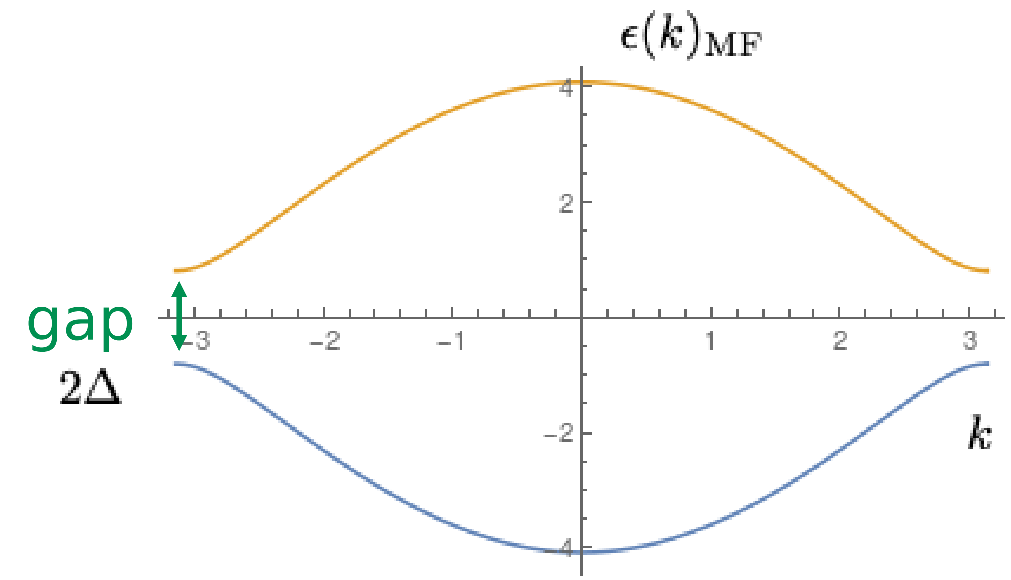
$$H = -\mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma} + t \sum_{ij,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$



$$\boxed{H_{\mathrm{MF}} = H_0 - U \sum_i M_i m_{iz}}$$

$$\boxed{M_i = \langle m_{iz} \rangle_{\mathrm{MF}}}$$





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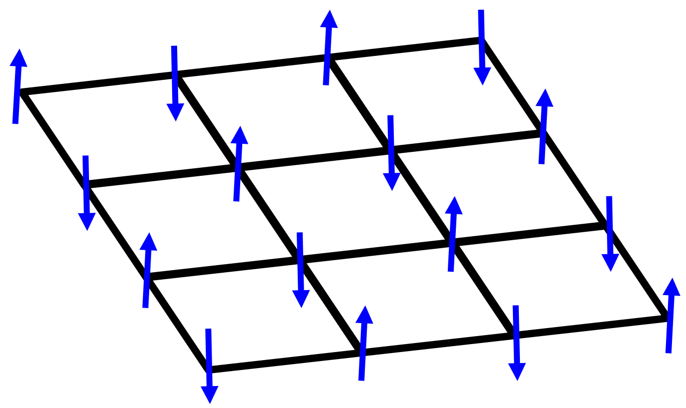

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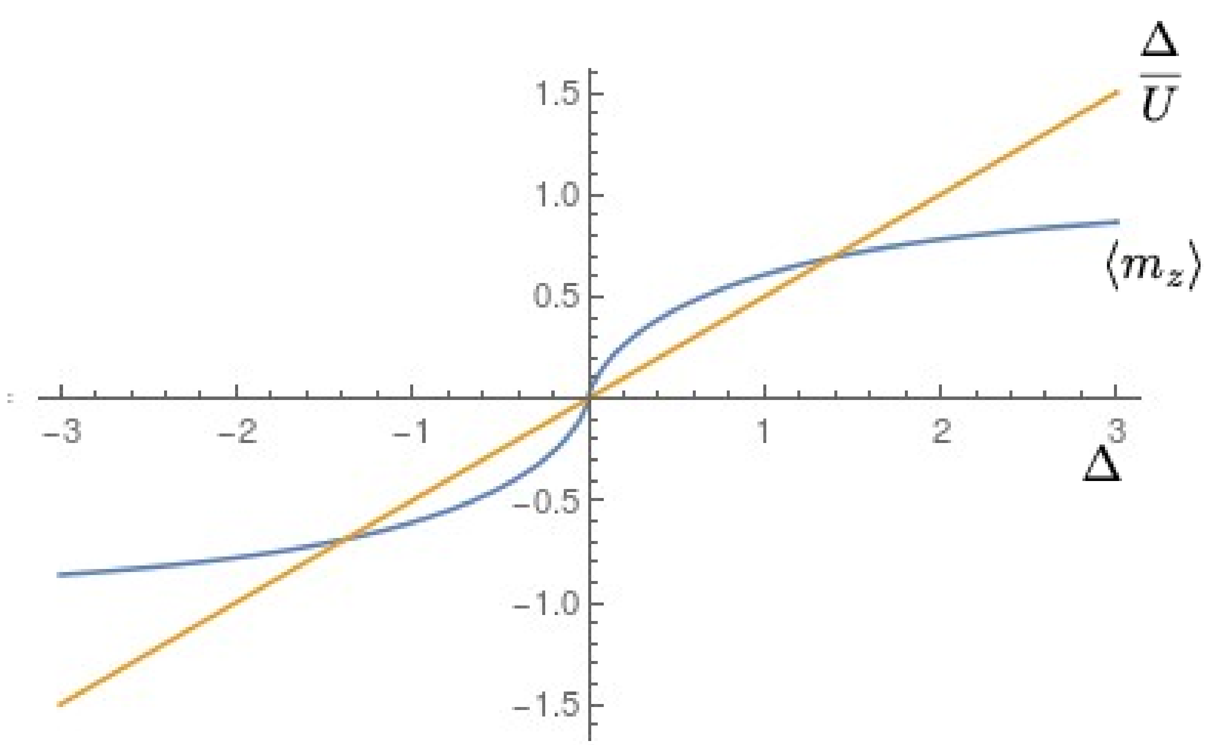

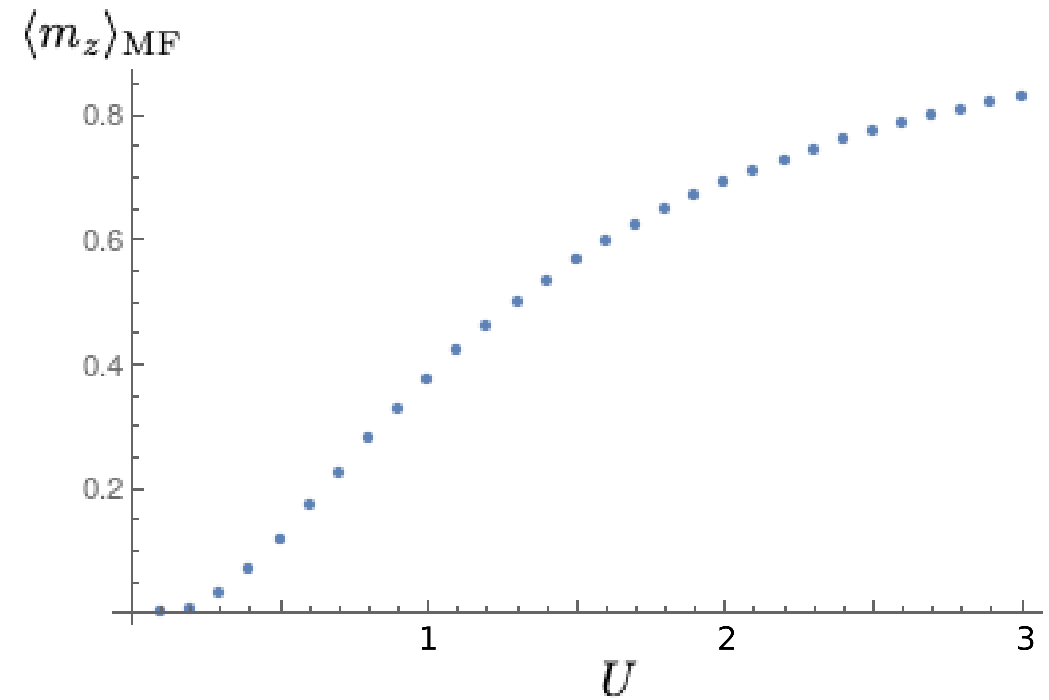

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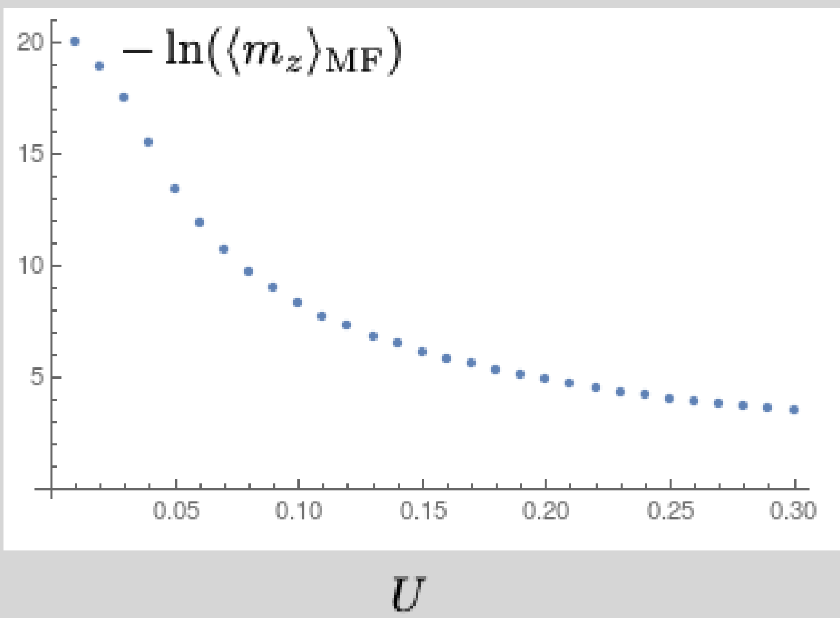
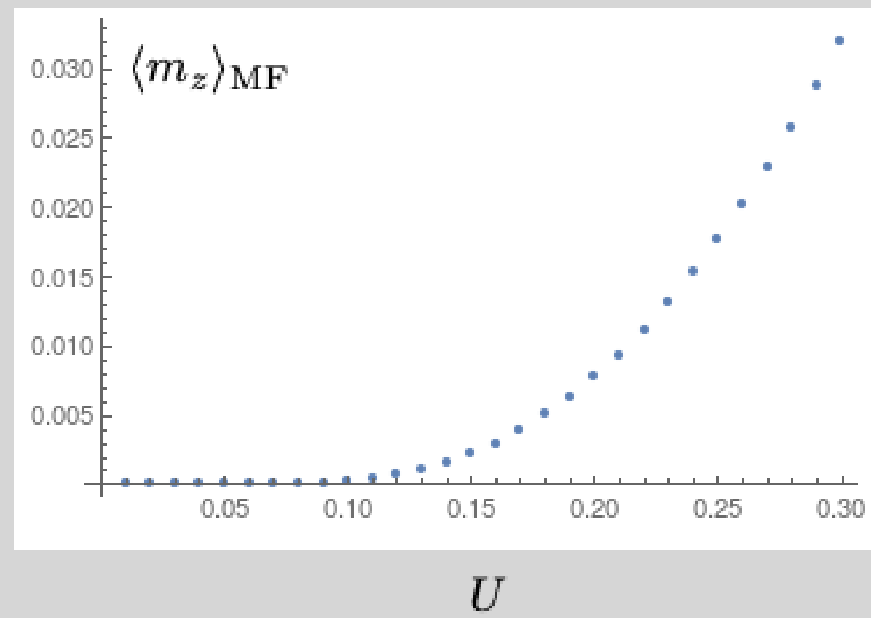
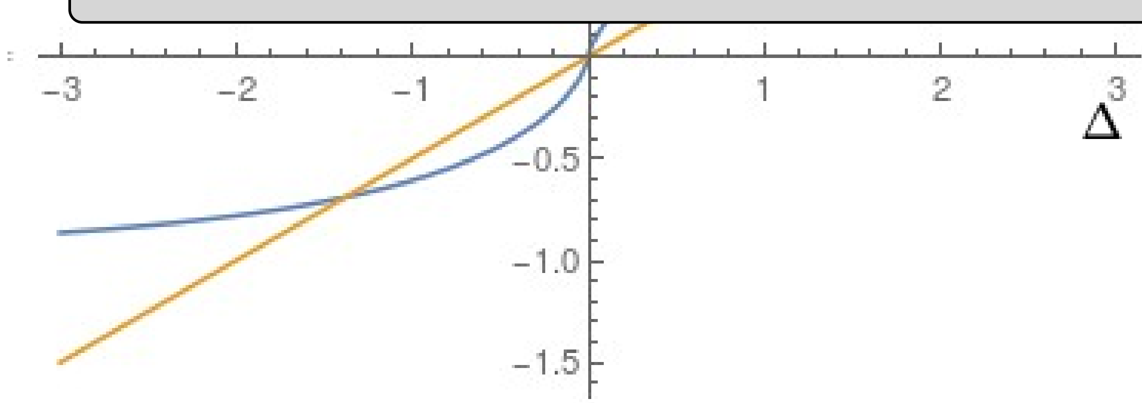
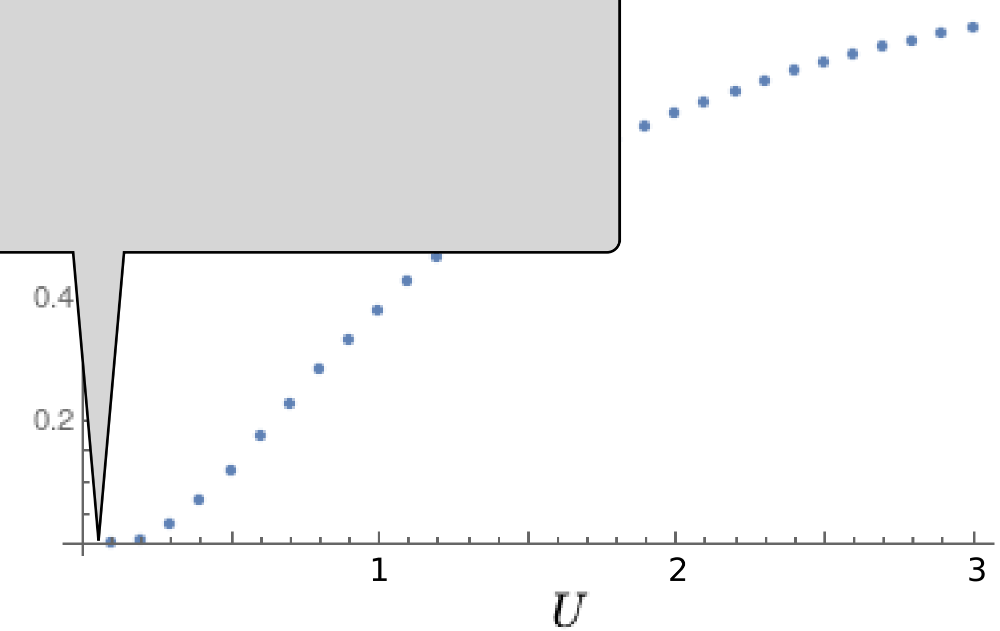
$M_i m_{iz}$



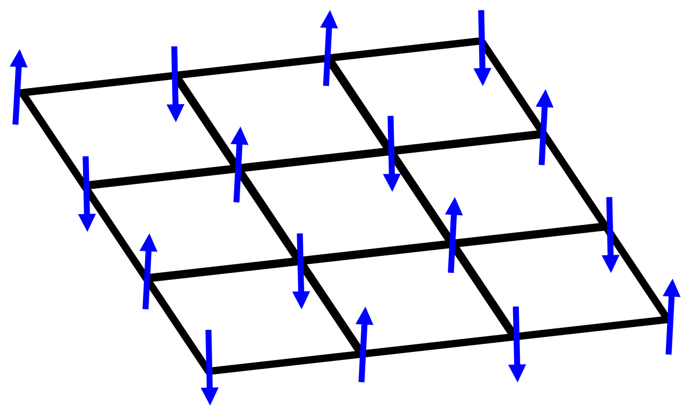


$$\ln(\langle m_z \rangle_{\mathrm{MF}}) \sim -\frac{1}{U}$$





Spontaneous symmetry breaking (mean-field theory)



The ground state breaks symmetries of the Hamiltonian:

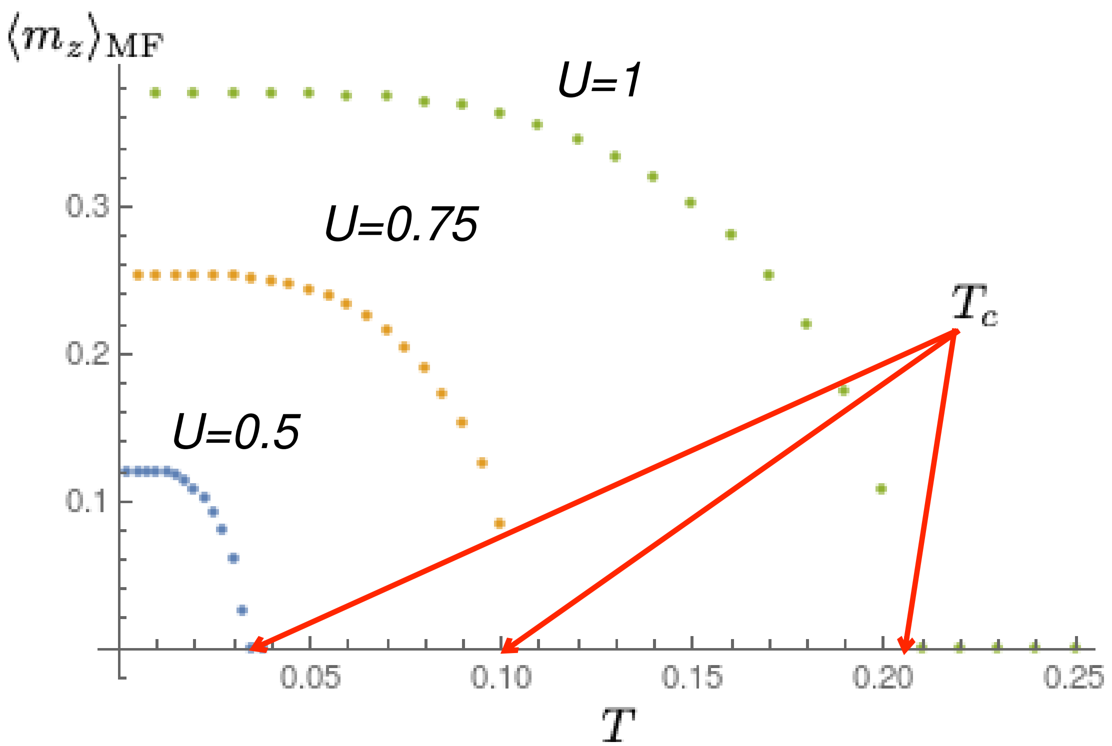
- spin isotropy (z-direction is special)
- periodicity (two sublattices)
- time-reversal

=> ground state is degenerate

=> if continuous symmetries are broken Goldstone modes
exist: magnons (FM, AFM), acoustic phonons (solids),
sound waves (BEC), ...

=> spontaneous symmetry breaking (second order phase transition) can exist only in infinite (macroscopic) systems

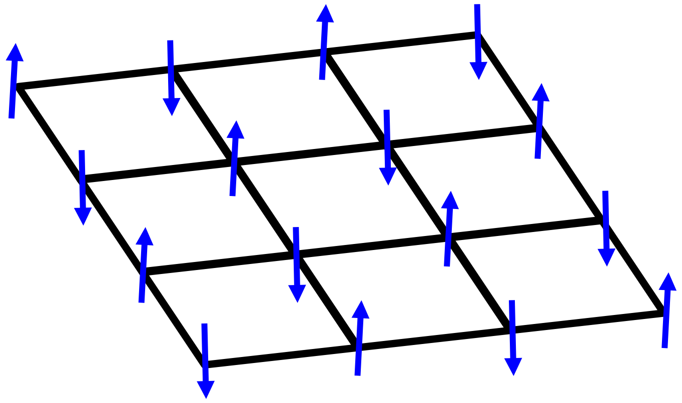
=> ordered phase is destroyed by temperature



Examples:
magnetic order (spin rotation symmetry)
crystalline order (translational symmetry)
superconductivity (particle conservation, gauge symmetry)
Bose-Einstein condensation (particle conservation, gauge symmetry)
charge/spin density waves (translational symmetry)

MF theory can be generalized to finite temperatures - it provides an accurate description
of spontaneous symmetry breaking in weak coupling limit, e.g. superconductivy

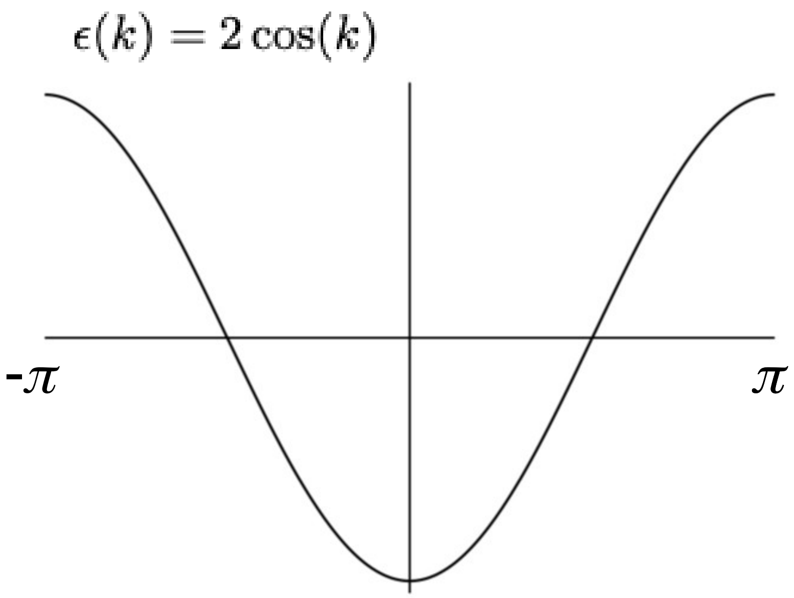
Spontaneous symmetry breaking (mean-field theory)

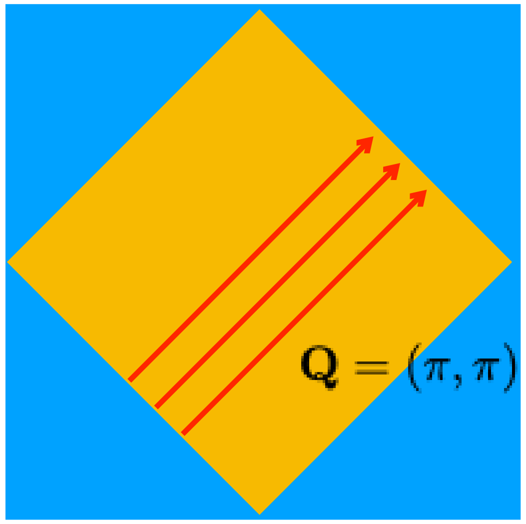


Why AFM and why the T=0 order exists for any U?

This is a special property of square lattice and half-filling!
(in generic case one gets an order at finite U if at all)

Perfect nesting of the Fermi surface:





Note the similarity with Peierls instability!
(However, perfect nesting is generic in 1D, but very special in 2D)