BCS-BEC crossover
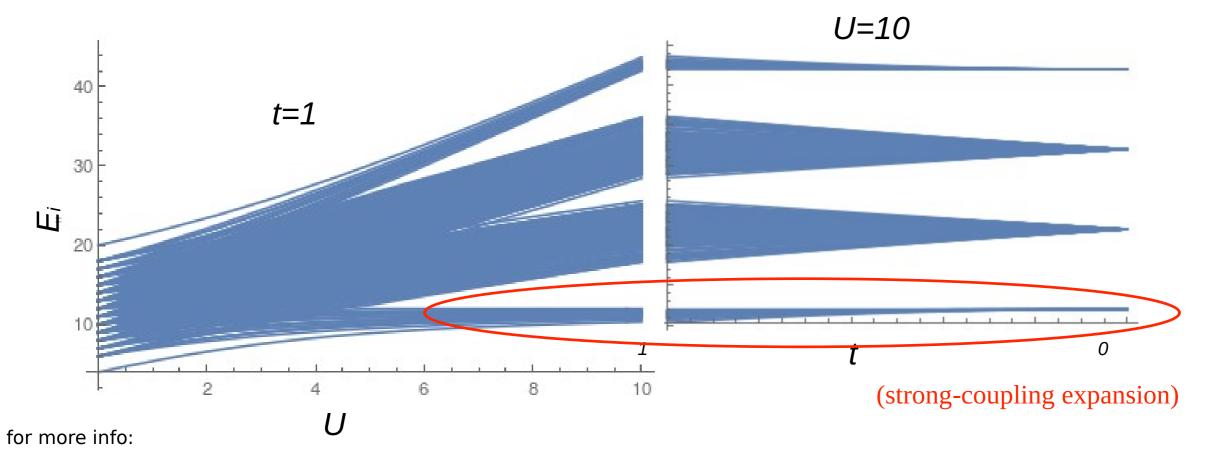
Formation of local moments

$$H = t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

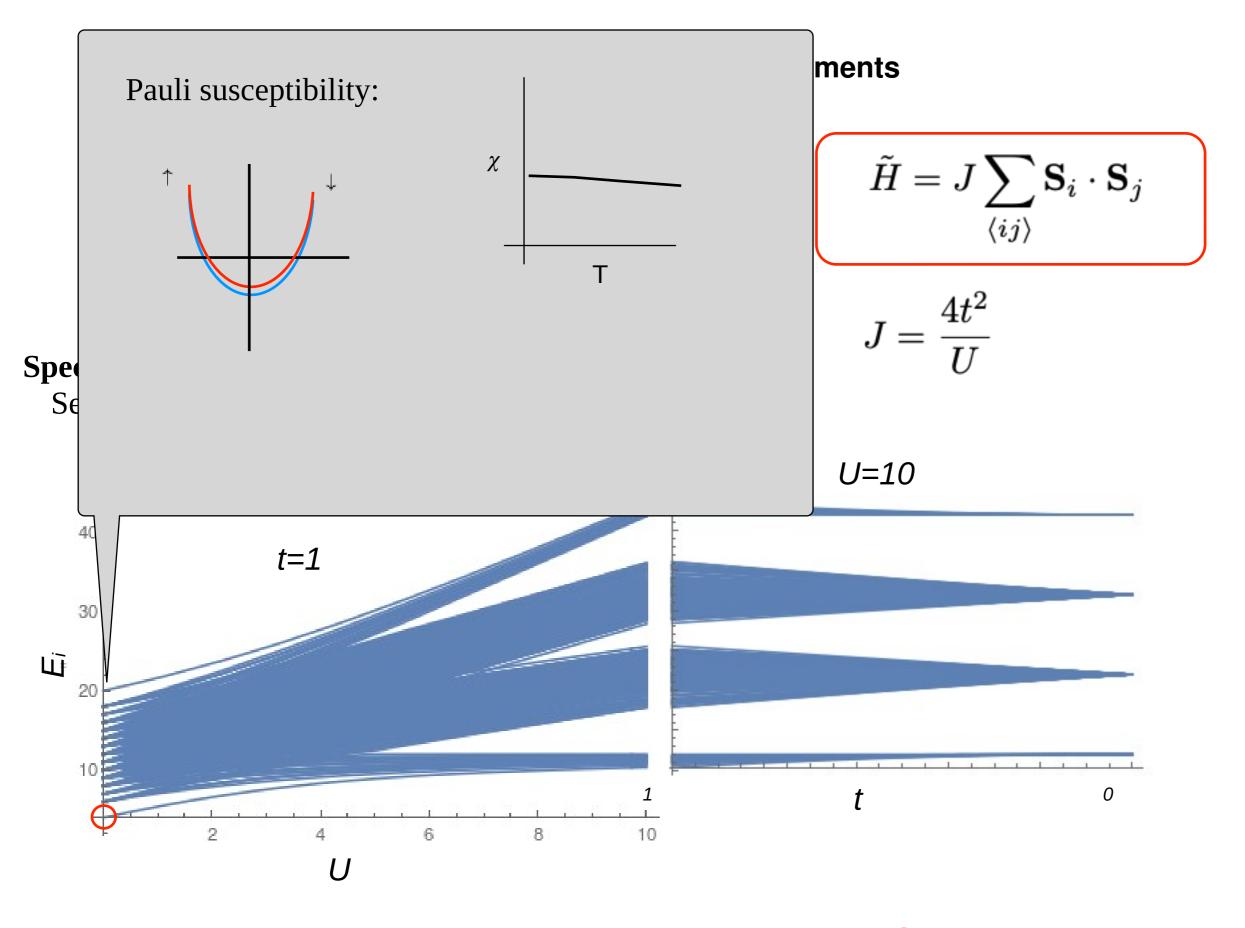$$\tilde{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$J = \frac{4t^2}{U}$$

Spectrum of eigenenergies (6-site Hubbard model):
Sector (3,3)
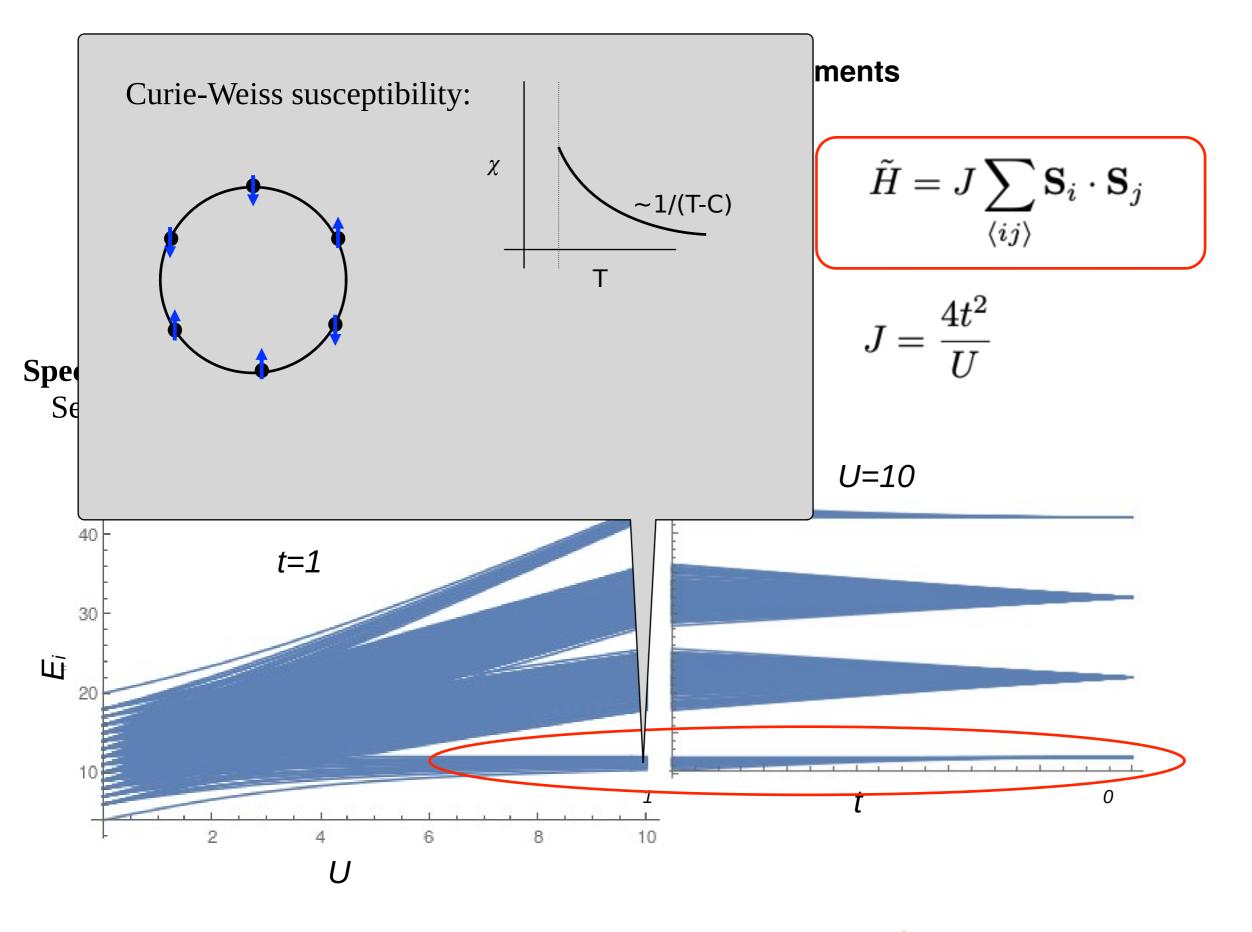
$U=10$

$t=1$

E_i

(strong-coupling expansion)

U

Beekman, Rademaker and van Wezel, SciPost Phys. Lect. Notes 11 (2019)

Pauli susceptibility:

χ

T

ments

$$\tilde{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$J = \frac{4t^2}{U}$$

U=10

Spe
Se

E_i

t=1

40

30

20

10

2   4   6   8   10

U

1

t

0

(strong-coupling expansion)

Curie-Weiss susceptibility:

χ

~1/(T-C)

T

ments

$$\tilde{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$J = \frac{4t^2}{U}$$

Spe
Se

$U=10$

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E_i

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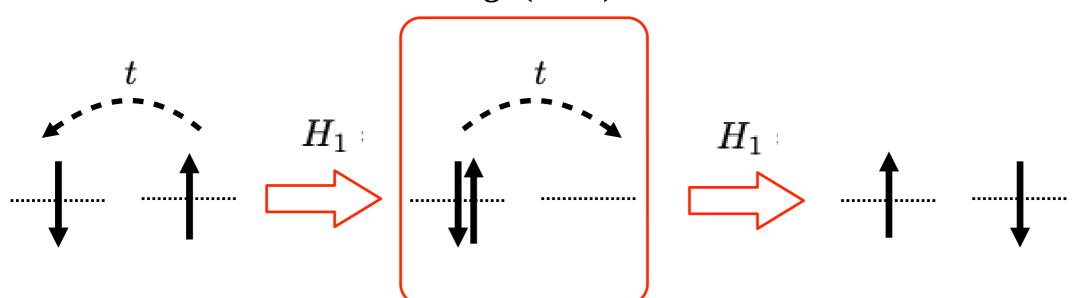2   4   6   8   10

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t

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(strong-coupling expansion)

Formation of local moments

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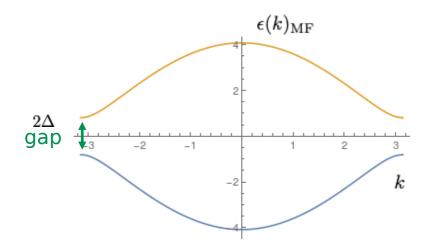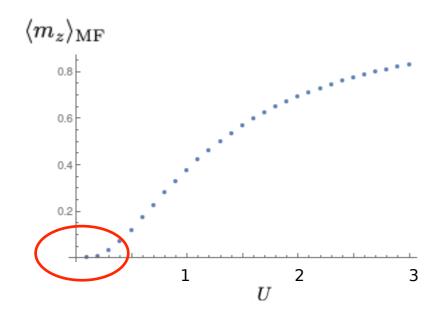
$$J = \frac{4t^2}{U}$$

U is large (U>>t)

$$\langle \alpha | H_{\mathrm{eff}} | \beta \rangle = \frac{1}{2} \sum_{\gamma} \left(\frac{\langle \alpha | H_1 | \gamma \rangle \langle \gamma | H_1 | \beta \rangle}{E_\alpha - E_\gamma} + \frac{\langle \alpha | H_1 | \gamma \rangle \langle \gamma | H_1 | \beta \rangle}{E_\beta - E_\gamma} \right)$$

BCS-BEC crossover

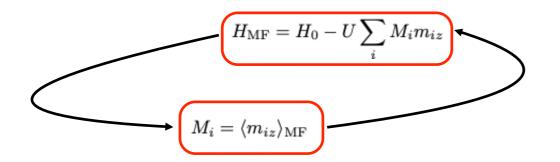$$H = -\mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \qquad M_i = (-1)^i M$$

weak-coupling limit:

strong-coupling limit:

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

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

$$\tilde{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

BCS-BEC crossover

$$H = -\mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \qquad M_i = (-1)^i M$$
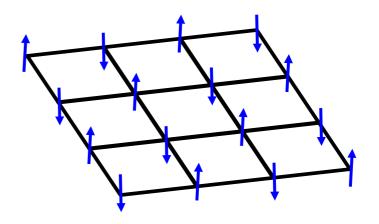
weak-coupling limit:

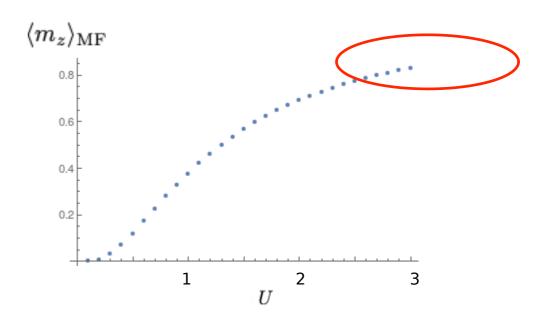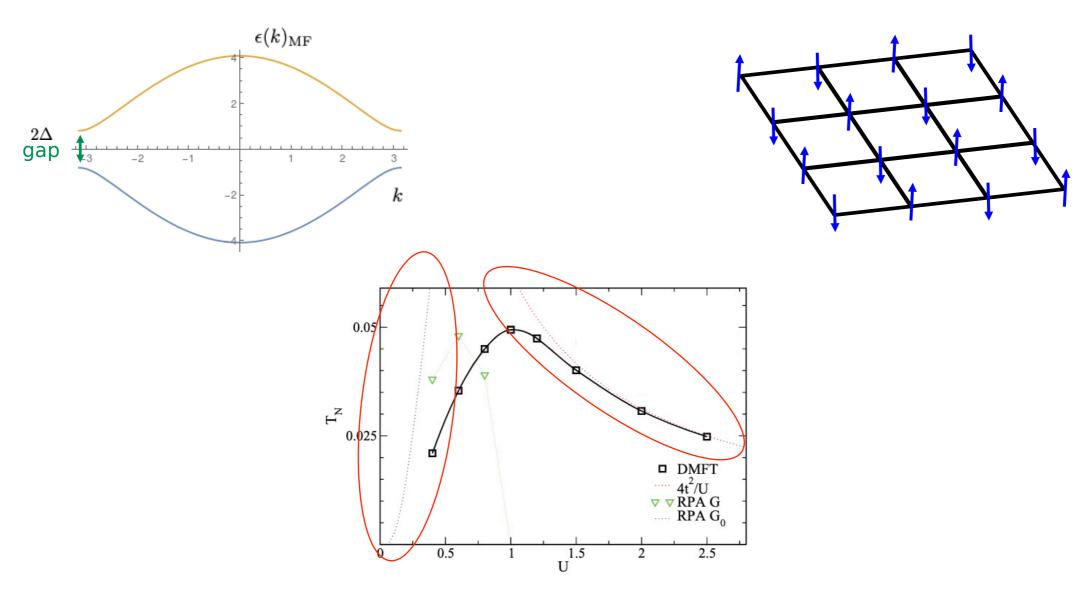strong-coupling limit:

$$T_N \sim N_q(0)U \sim \frac{U}{D}$$

$$T_N \sim \frac{t^2}{U}$$

BCS-BEC crossover

$$H = -\mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \qquad M_i = (-1)^i M$$
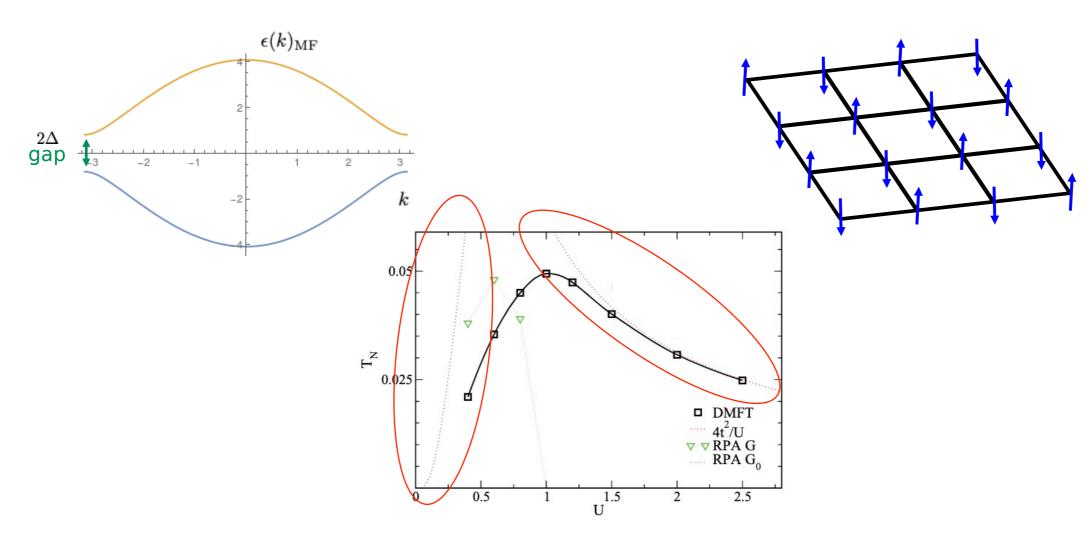
weak-coupling limit:

strong-coupling limit:

Bethe-Salpeter equation: $\qquad \chi = \chi_0 + \chi_0 \Gamma \chi \qquad \chi = (I - \chi_0 \Gamma)^{-1} \chi_0$

BCS-BEC crossover

$$H = -\mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \qquad M_i = (-1)^i M$$

weak-

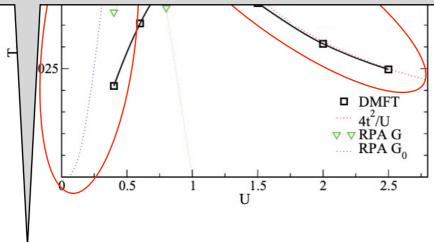$$\chi(Q; q_1, q_2) = \chi_0(Q; q_1, q_2) + \chi_0(Q; q_1, \bar{k}_1)\Gamma(Q; \bar{k}_1, \bar{k}_2)\chi(Q; \bar{k}_2, q_2)$$

physical susceptibility:
$$\chi(Q) = T \sum_{q_1, q_2} \chi(Q; q_1, q_2)$$

'bubble'
$$\chi_0(Q; q_1, q_2) = \delta_{q_2, q_1+Q} G(q_1) G(q_1 + Q)$$

frequency & momentum
$$q = (\omega, \mathbf{q})$$
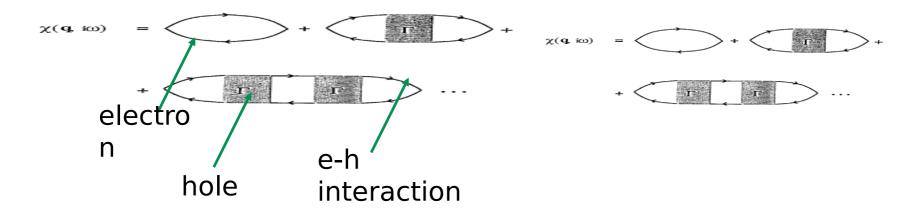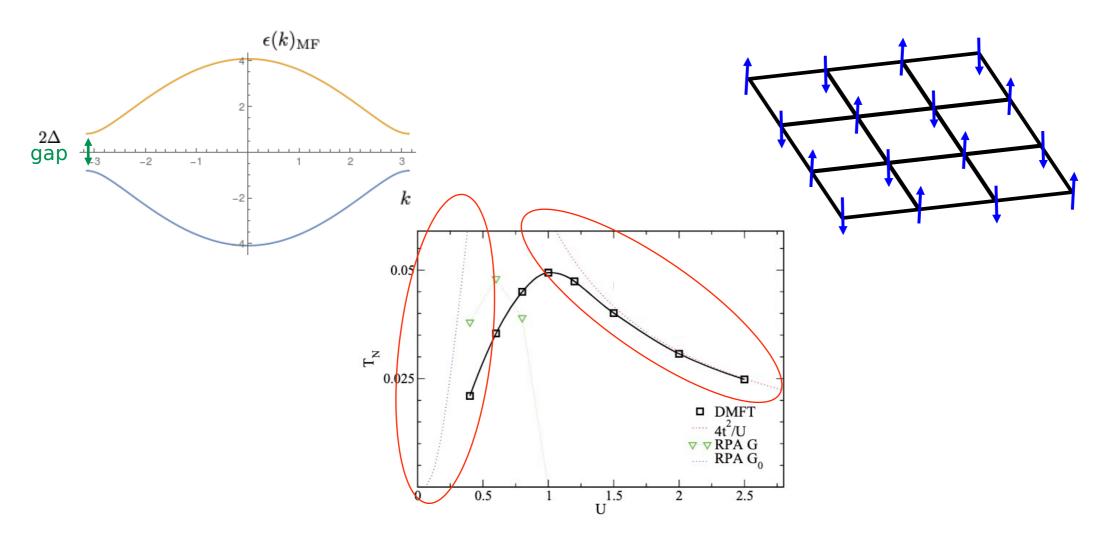
static response
$$Q = (0, \mathbf{Q})$$

025

- ▢ DMFT
- ⋯⋯ $4t^2/U$
- ▽ ▽ RPA G
- ⋯⋯ RPA G_0

0   0.5   1   1.5   2   2.5

U

Bethe-Salpeter equation: $\chi = \chi_0 + \chi_0 \Gamma \chi$ $\chi = (I - \chi_0 \Gamma)^{-1} \chi_0$

electron

hole

e-h interaction

BCS-BEC crossover

$$H = -\mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \qquad M_i = (-1)^i M$$

weak-coupling limit:

strong-coupling limit:

Bethe-Salpeter equation: $\qquad \chi = \chi_0 + \chi_0 \Gamma \chi \qquad \chi = (I - \chi_0 \Gamma)^{-1} \chi_0$

RPA (random phase approximation) $\qquad\qquad\qquad\qquad$ Atomic vertex

$$\Gamma \approx U$$

$$\chi_0(T_c) U = I$$

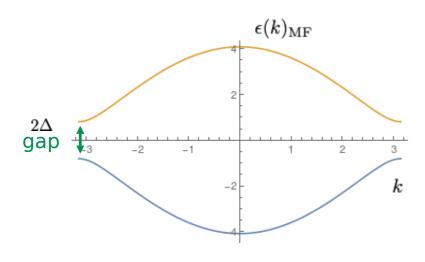Transition is driven by the T-dependence of the 'bubble' $\qquad\qquad\qquad$ Transition is driven by the T-dependence of the vertex
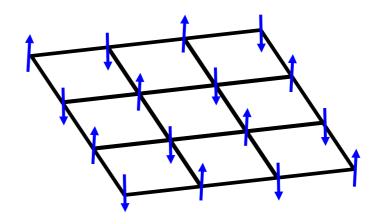
BCS-BEC crossover

$$H = -\mu \sum_{i,\sigma} c_{i\sigma}^\dagger c_{i\sigma} + t \sum_{ij,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \qquad M_i = (-1)^i M$$

weak-coupling limit:

strong-coupling limit:

Normal phase: excitation - almost independent quasiparticles
=> broad peaks, dispersion apparent only close
to the transition

Ordered phase: only 1P states close to FL affected
=> large spatial extent of the 'condensed
particles'

Superconductivity: Cooper pairs absent in normal phase
CPs have large spatial extent
(many CPs overlap)

excitation - strongly bound pairs of QP
=> exist well above T_c, the formation T
and transition T are very different
Curie susceptibility 1/T

excitations condense = become coherent
(local moments point in fixed direction)
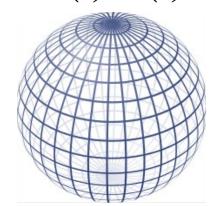
Mott antiferromagnetism, exciton condensation

Spontaneous symmetry breaking

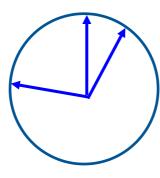3D magnet   planar magnet

Symmetry group *G* of the Hamiltonian:

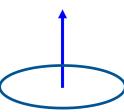*SO(3)~SU(2)*   *SO(2)=U(1)*

Order parameter and residual symmetry (symmetry of the ground state) *H*:

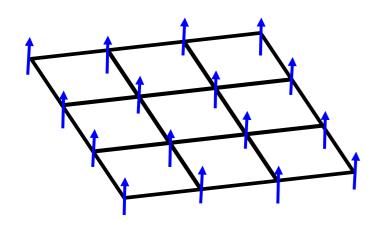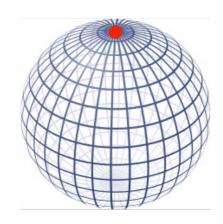*U(1)*   *{I}*

Set of all possible order parameters *G/H* (coset of G not necessarily a group):

S_2 $U(1)=S_1$

Spontaneous **symmetry** breaking

S=1

$$H = -J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

Spontaneous **symmetry** breaking

S=1
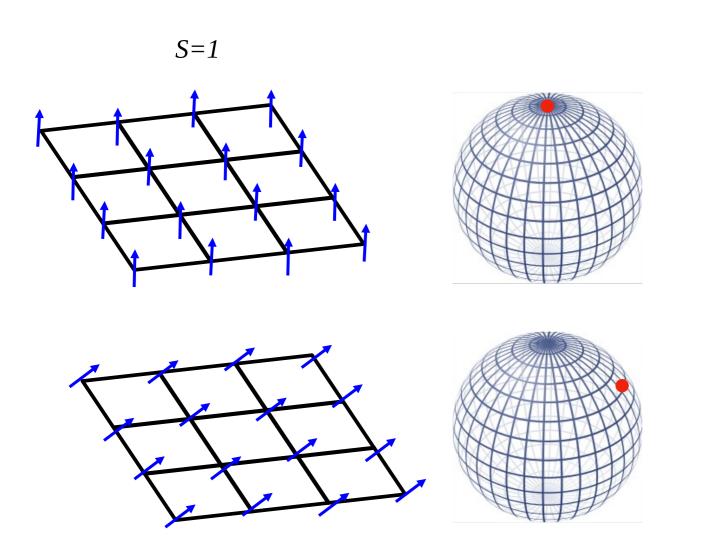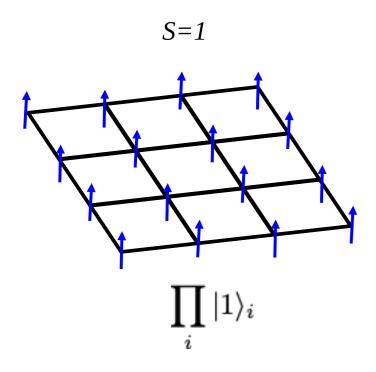
$$H = -J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

The same order (a different ground state obtained by an operation from *G/H* - orthogonal and degenerate with the above state).

Can we get a different ordered state (assuming uniform order)?

Spontaneous **symmetry** breaking

S=1

$$\prod_i |1\rangle_i$$

$$H = -J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

Yes!

$$\prod_i |0\rangle_i$$

$$H = -J \sum_{ij} \left[\mathbf{S}_i \cdot \mathbf{S}_j + 4(\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 2(\mathbf{S}_i \times \mathbf{S}_j)^2 \right]$$

There is no *SU(2)* rotation that takes |1> to |0>

Dimensionality

Examples: correlations in everyday life

any D - Coulomb blockade: "in a crowded gym you are stuck
at one station"

Dimensionality

Examples: correlations in everyday life
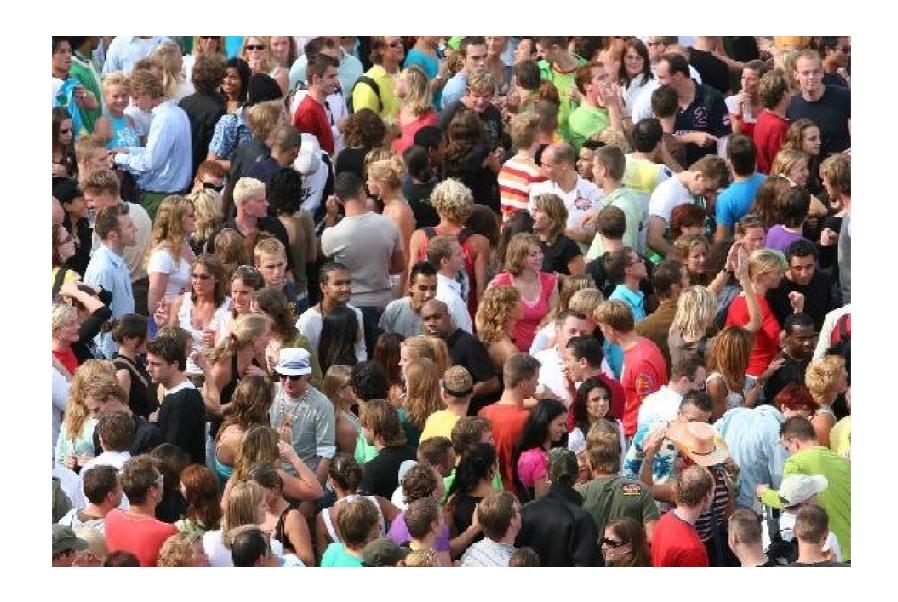
1D - complete loss of individual identity

Dimensionality

Examples: correlations in everyday life

2D - fading through a crowd "you become heavy"

Density of states

Definition:

$$D(\omega) = \frac{1}{N} \sum_{n,\mathbf{k}} \delta(\omega - \epsilon_{\mathbf{k}n})$$

$$= \frac{\Omega}{(2\pi)^3} \sum_n \int_{BZ} d^3k \quad \delta(\omega - \epsilon_n(\mathbf{k})) = \frac{\Omega}{(2\pi)^3} \sum_n \int_{\epsilon_n(\mathbf{k})=\omega} \frac{dS}{|\nabla_k \epsilon_n(\mathbf{k})|}$$

Calculation:

- histogram (brute force summation over discrete k-mesh)

  'trick': use $\delta(\omega - \epsilon) = -\frac{1}{\pi} \text{Im} \lim_{\Gamma \to 0} \frac{1}{\omega - \epsilon + i\Gamma}$ and perform the calculation for small finite Γ.

- analytic calculation - band edges (van Hove singularities)

  The states with $\epsilon(\mathbf{k}) - \epsilon_0 \sim k^2$ and $\epsilon(\mathbf{k}) - \epsilon_0 < \omega$ live in a k-sphere of radius $\omega^{1/2}$

  This gives rise to characteristic behavior close to the band edge:

	$N(\omega)$	$D(\omega)$
1D	$\omega^{1/2}$	$\omega^{-1/2}$
2D	ω	1
3D	$\omega^{3/2}$	$\omega^{1/2}$

Density of states

Definition:

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$$= \frac{\Omega}{(2\pi)^3} \sum_n \int_{\text{BZ}} d^3k \ \ \delta(\omega - \epsilon_n(\mathbf{k})) = \frac{\Omega}{(2\pi)^3} \sum_n \int_{\epsilon_n(\mathbf{k})=\omega} \frac{dS}{|\nabla_k \epsilon_n(\mathbf{k})|}$$

Calculation:
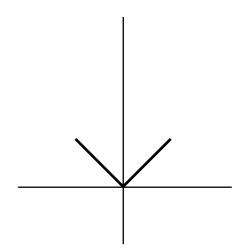- histogram (brute force summation over discrete k-mesh)
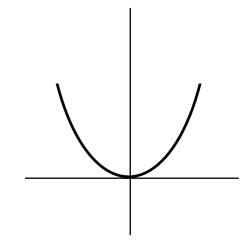
  'trick': use $\delta(\omega - \epsilon) = -\frac{1}{\pi} \text{Im} \lim_{\Gamma \to 0} \frac{1}{\omega - \epsilon + i\Gamma}$ and perform the calculation for small finite .
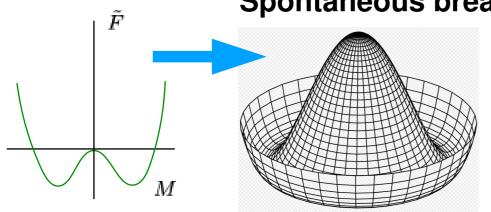
- analytic calculation - band edges (van Hove singularities)

  The states with $\epsilon(\mathbf{k}) - \epsilon_0 \sim k$ and $\epsilon(\mathbf{k}) - \epsilon_0 < \omega$ live in a k-sphere of radius ω

  This gives rise to characteristic behavior close to the band edge:

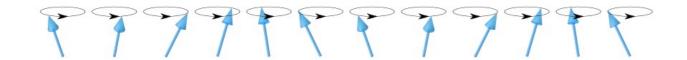|	$N(\omega)$	$D(\omega)$
1D	ω^1	1
2D	ω^2	ω
3D	ω^3	ω^2

Spontaneous breaking of continuous symmetry

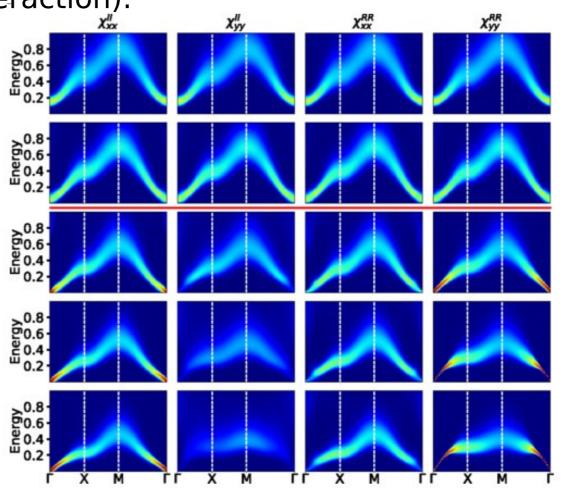Continuous symmetries: space isotropy (orbital or spin rotations),
space isotropy (translation), gauge symmetries (charge conservation)

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

Spontaneous breaking of continuous symmetry

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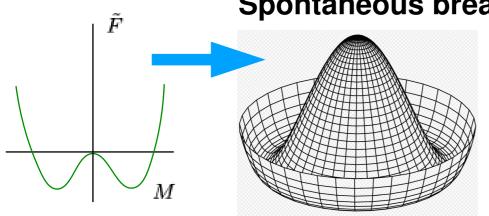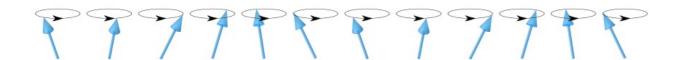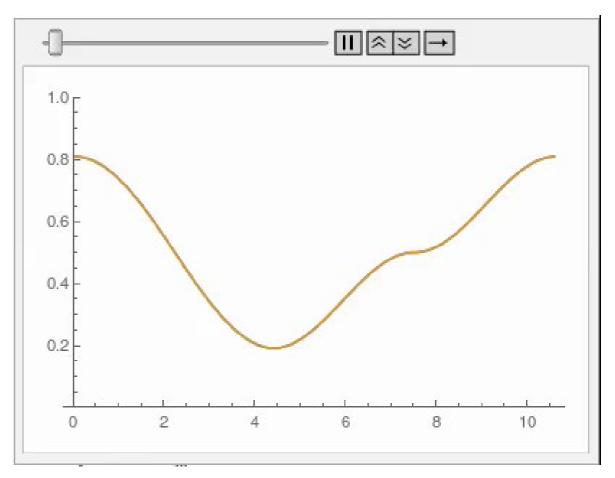2 linear modes in 2-orbital Hubbard model (exciton condensate phase)

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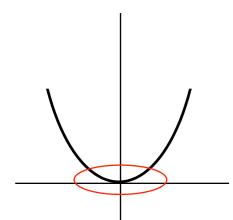normal gas -> Bose-Einstein condensate

Goldstone mode

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

Absence of order in low dimensions

Ferromagnet: ↑↑↑↑↑↑↑↑↑↑↑↑ exact groundstate

excitations: $|k\rangle = $ ↓↑↑↑↑↑↑↑↑↑↑↑ $+e^{ik}$ ↑↓↑↑↑↑↑↑↑↑↑↑ $+e^{i2k}$ ↑↑↓↑↑↑↑↑↑↑↑↑ magnon

Thermal population of magnons reduced the ordered moment M.
If 'many' magnons are populated M can completely vanish. How many magnons are populated depends on the density of states (dispersion + dimension).

Antiferromagnet: ↑↓↑↓↑↓↑↓↑↓↑↓ ⇌ ↑↓↑↓↑↓↑↑↑↓↑↓↑↓

quantum fluctuations (T=0)

The Neel state is only approximate ground state. Can the quantum fluctuations destroy it?
The answer is yes in 1D. In D=2 or 3 quantum corrections are finite and only reduce the ordered moment.

AFM magnons destroy the Neel order in 2D for T>0.

Absence of order in low dimensions

Antiferromagnet - quantum correction:

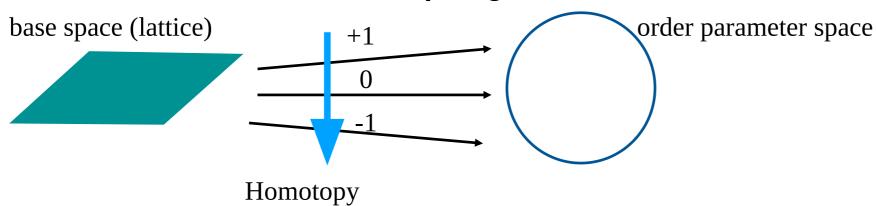| $\langle N^z \rangle / N$	absolute	relative	$S = \frac{1}{2}$		$S = 1$	
$D = 2$	$S - 0.1966$	$19.7/S$ %	0.303	39.3%	0.803	19.7%
$D = 3$	$S - 0.0784$	$7.8/S$ %	0.422	15.6%	0.922	7.8%

Antiferro-, ferro- and ferrimagnet at T=0 and T>0
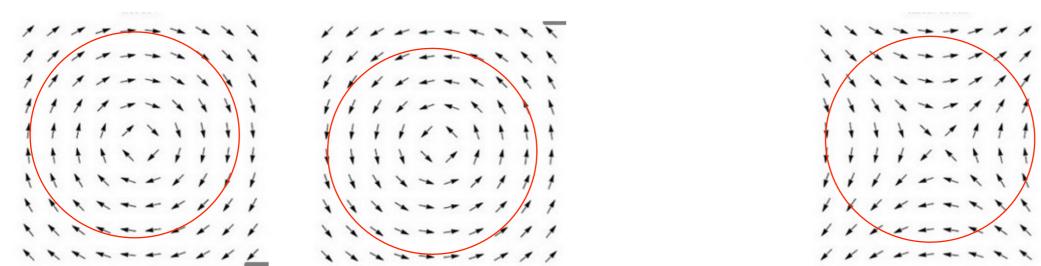
	NG mode dispersion	ground state degeneracy	tower of states	quantum corrections	lower critical dimension	
					$T = 0$	$T > 0$
type-A	$\propto k$	no	yes	yes	1	2
type-B ferro	$\propto k^2$	yes, $\mathcal{O}(N)$	no	no	0	2
type-B ferri	$\propto k^2, M + k^2$	yes, $\mathcal{O}(N)$	no	yes	0	2

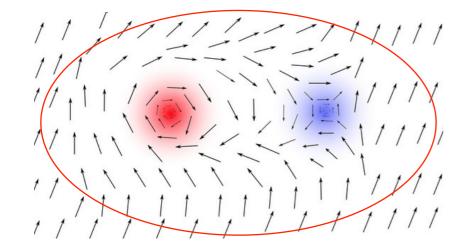Beekman, Rademaker and van Wezel, SciPost Phys. Lect. Notes 11 (2019)

Topological excitations

base space (lattice)

+1

0

-1

order parameter space

Homotopy

vortex: +1

antivortex: -1

vortex-antivortex pair:

Kosterlitz–Thouless transition

- 2D xy-model
- no local order parameter
- normal phase (exp correlations), ordered phase (power law correlations)
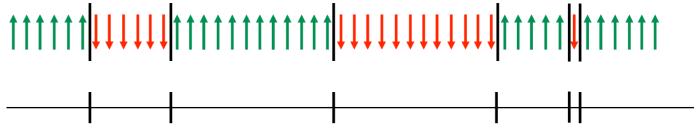- unbinding of vortex-anti-vortex pairs

Lack of order in 1D, T>0

$$H = -J \sum_{ij} S_i^z S_j^z, \quad S_z = \pm 1 \qquad \text{Ising model}$$

T=0, exact ground state: ↑↑↑↑↑↑↑↑↑↑↑↑ or   ↓↓↓↓↓↓↓↓↓↓↓↓

excitations: (gapped) *E=2J*   ↑↑↑↑↑↓↑↑↑↑↑↑   ↑↑↑↑↑↑↑↑↑↓↑↑↑

excitations: (gapped) *E=J*   ↑↑↑↑↑↑|↓↓↓↓↓↓

T>0, typical state (<S>=0 no order):   ↑↑↑↑↑↑|↓↓↓↓↓↓|↑↑↑↑↑↑↑↑↑↑↑↑|↓↓↓↓↓↓↓↓↓↓↓↓|↑↑↑↑↑|↑↑↑↑↑↑

What makes 1D different?

The surface does not depend on the volume.
=> growing a domain with 'opposite' order costs finite energy independent of the domain size

=>@T>0 there is always a finite probability do find the domain wall(s)

=> correlation length depends on the concentration of domain walls, finite concentration of
   domain walls implies a finite correlation length