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MINIWORKSHOP ON STRONG ELECTRON CORRELATIONS
"Disorder and Interaction in Quantum Systems and Their Classical Analogs"

(1 - 19 July 1996)

"Collective screening of quantum spins by phonons; a possible scenario for Heavy Fermions"

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These are preliminary lecture notes, intended only for distribution to participants.

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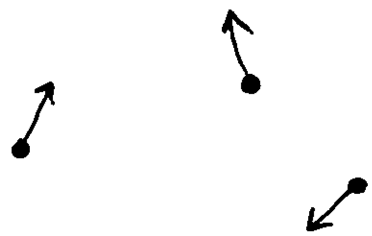
Collective screening of quantum spins by phonons;
a possible scenario for Heavy Fermions

H. Capellmann
A.I.

Contents

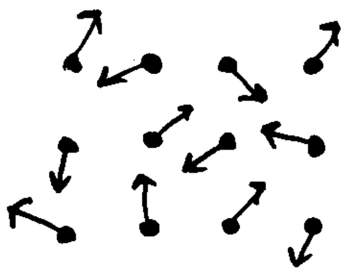
Magnetic ions in metals



Alloy or regular lattice

Localized
d-electrons (Transition metals ...)
or
f-electrons (Rare Earths Actinides ...)

High $T > T_c$



Paramagnet

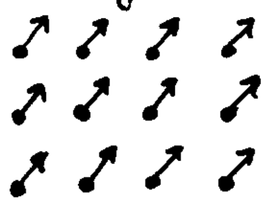
Spins are freely rotating.
T-invariant state

Curie Law:

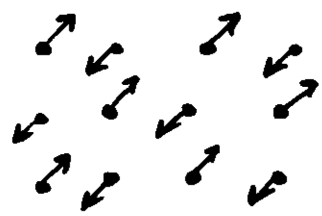
$$\chi \sim 1/T$$

Low $T < T_c$

Magnetic order:



Ferromagnet

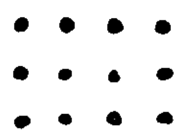


Antiferromagnet

Broken T-invariance
magnetic ground state
with quenched spins

NOT ALWAYS!

Sometimes:
nonmagnetic ground state
(e.g. heavy fermion compounds)

??  no magnetic order.

Interactions of localized spins

With each other

with conduction electrons

with phonons

RKKY

Kondo effect

Effective Spin-spin Interaction

Screening of individual spins

Collective effects (nonperturbative)

Competition

Magnetic ground state

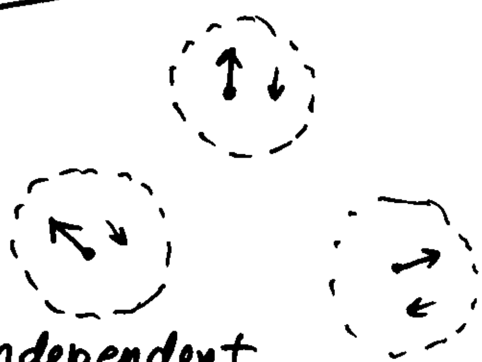
nonmagnetic ground state

Most magnetic crystals.

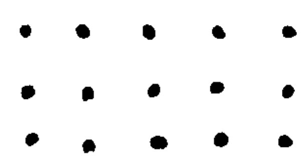
$$\hat{H} = \sum_{aa'} J_{aa'}^{\alpha\alpha'} S_a^\alpha S_{a'}^{\alpha'}$$

Diluted magnetic alloys

Some heavy-fermion compounds



Independent Kondo-singlets



?? Still a puzzle

Important notes for a dense lattice of spin.

- Weak Coupling $\rightarrow$ Effective Spin-Hamiltonian $\rightarrow$ Magneti Order

- Nonmagnetic ground state may only be possible for strong coupling:

  $J > J_c$ (certain threshold)

- **Nonperturbative approach is absolutely necessary**
- **Collective effects are important**

- Kondo-lattice scenario (only conduction electrons) has difficulties:

  J_c is large ($\sim 10^3$-10^4K) while T_c should be small ($\sim$1-10K)

- Although phonons can not screen a single half-integer spin (Kramers Theorem) the screening may occur due to the Collective effects.

Spin - Phonon Scenario

$$H = H_{ph} + H_{int}$$

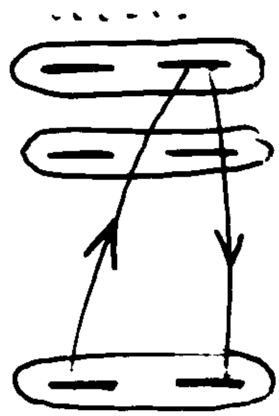
Hamiltonian of phonons:

$$H_{ph} = \sum_{b} \frac{1}{2M_b} \left(P_b^{\beta} \right)^2 + \frac{1}{2} \sum_{bb'} U_{bb'}^{\beta\beta'} Q_b^{\beta} Q_{b'}^{\beta'}$$

Effective spin - two phonon interaction:

$$H_{int} = \sum_{abb'} K_{abb'}^{\alpha\beta\beta'} S_a^{\alpha} Q_b^{\beta} P_{b'}^{\beta'}$$

Microscopic origin of H_{int}

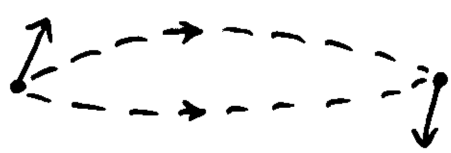


Interaction with phonon-induced fluctuation of crystal field.

Second order process

Perturbation Theory ($K \ll \omega$ - phonon energy)

$$H \xrightarrow[\text{phonons}]{\text{excluding}} H_{eff} = \sum_{aa'} \tilde{J}_{aa'}^{\alpha\alpha'} S_a^{\alpha} S_{a'}^{\alpha'} \quad \text{with } J \sim \frac{K^2}{\omega}$$



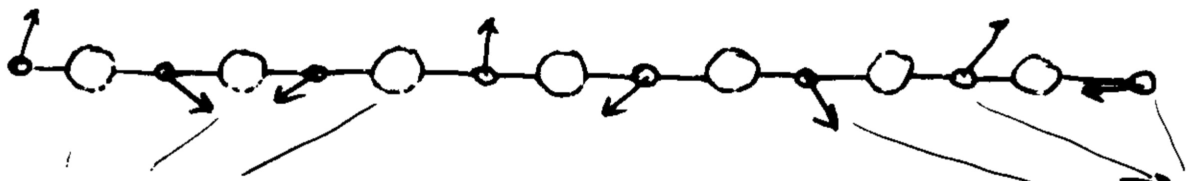
Exchange of two phonons

In heavy fermion compounds H_{int} is strong:

$$K \sim 100K \sim \omega$$

Nonperturbative treatment is possible only for model H

The Basic Model



3-component isotropic oscillators $\vec{Q}_b$:

Spins $\vec{S}_a$ $(s = 1/2)$

$$V^{\beta\beta'}_{bb'} = \delta_{bb'}\delta_{\beta\beta'}\omega^2$$

Nearest neighbour interaction with high symmetry

$$K^{\alpha\beta\beta'}_{abb'} = K\,\epsilon_{\alpha\beta\beta'}\,\delta_{bb'}\,\delta_{\langle ab\rangle}$$

$$\boxed{H = \frac{1}{2}\sum_b \vec{P}_b^2 + \omega^2\vec{Q}_b^2 + K\sum_{\langle ab\rangle}(\vec{S}_a\vec{L}_b)}$$

where $\vec{L}_b = [\vec{Q}_b, \vec{P}_b]$ oscillators angular momentum.

"Effective spin-orbit"

In this model the ground state can be found explicitly for arbitrary K

Infinite set of conservation laws:

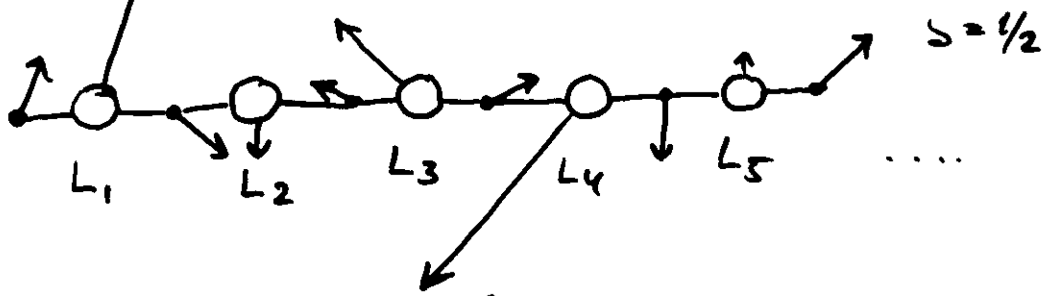
for any ℓ $\vec{L}_\ell^{\,2}$ commutes with $\hat{H}$,

<u>$\{L_\ell\}$ are good quantum numbers.</u>

In each sector, characterized by $\{L_\ell\}$:

$$H\{L_\ell\} = \sum_\ell \omega L_\ell + K \sum_{\langle a\ell\rangle} (\vec{S}_a \vec{L}_\ell) \quad ; \quad \vec{L}_\ell^{\,2} = L_\ell(L_\ell+1)$$

Effective Heisenberg model with spins of variable length:



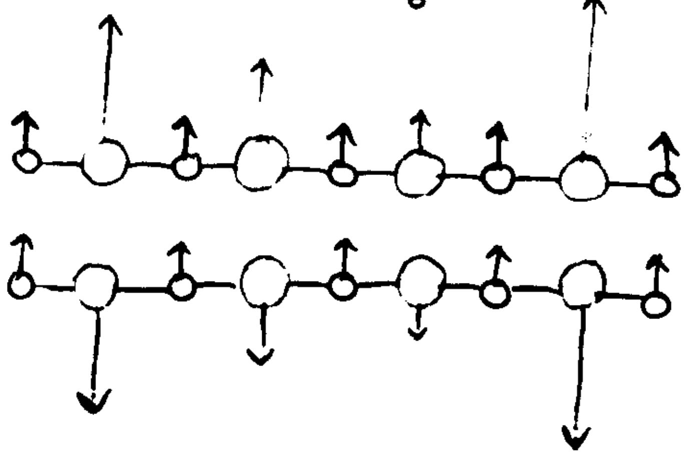
<u>In principle:</u>

1. Solve for any given $\{L_\ell\}$ and find the ground state $\Psi_G\{L_\ell\}$
2. Minimize $E_G\{L_\ell\}$ with respect to $\{L_\ell\}$.

<u>It is unrealistic</u>

Fortunately the actual set $\{L_\ell\}_{\text{Ground}}$ is very simple; and allow for an exact solution

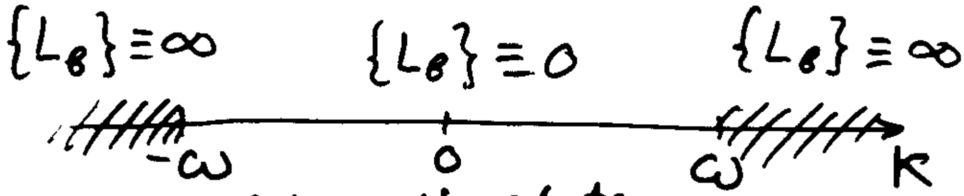
For classic vectors $\vec{L}_\ell$ in the ground state:

either  (for $K<0$)

or (for $K>0$)

and $E_G\{L_\ell\} = \underline{(\omega-|K|)\sum_\ell L_\ell} + \text{Quantum Correct}$

<u>Classic phase diagram</u>

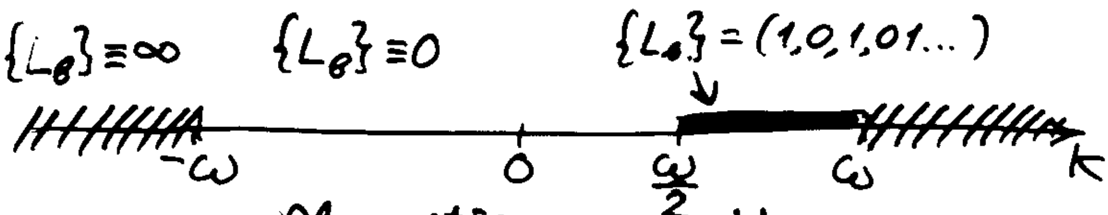


Magnetic state
oscillators are
not excited
Spins are free.

Lattice instability

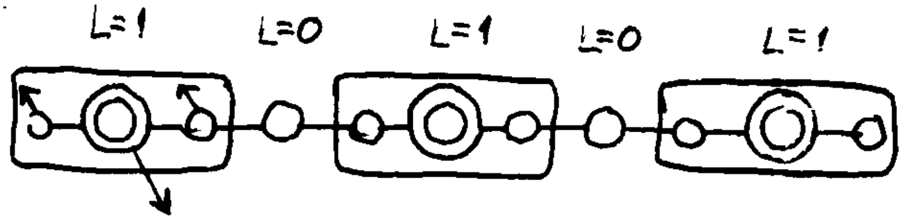
Close to the instability point $K=\omega$, where $E_G^{class}\{L_\ell\}\to 0$ Quantum Corrections must dominate:

<u>Quantum (exact) phase diagram</u>



Magnetic state

Nonmagnetic state



Singlet spin-phonon complexes (dimers)

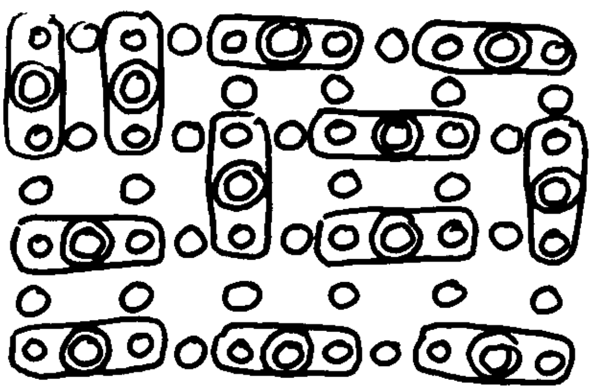
$$H_{dimer} = \omega L + K(\vec{L}(\vec{S}_1 + \vec{S}_2))$$

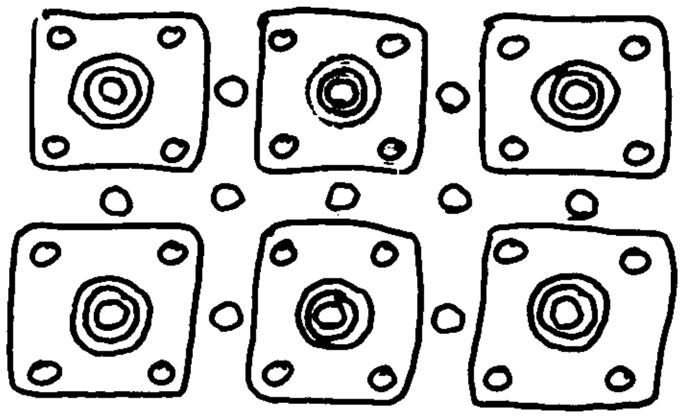
In the ground state: $L = 1$ $S = 1$ $J = 0$
for $\frac{\omega}{2} < K < \omega$

$(\vec{S} = \vec{S}_1 + \vec{S}_2)$ $(\vec{J} = \vec{L} + \vec{S}_1 + \vec{S}_2)$

No interaction between dimer in Basic Model

Generalization for higher dimensions and higher spins

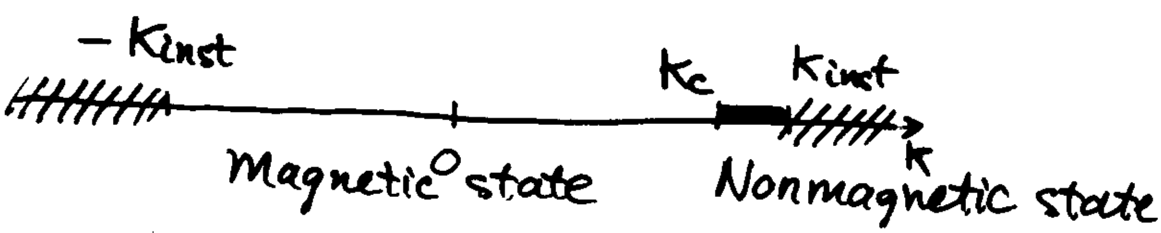




spin s, coordination number z

$$H_{complex} = \omega L + K(\vec{L}(\vec{S}_1 + \vec{S}_2 + \dots \vec{S}_z))$$

Ground state: $L = sz$, $S = sz$, $J = 0$



Nonmagnetic states in the Basic Model

- Nonperturbative effect: occurs only in a certain range of coupling constants: $K_c < K < K_{inst}$

- Quantum effect: no classic displacements: $\langle Q_\theta \rangle \equiv 0$, only the amplitude of zero vibrations $\langle Q_\theta^2 \rangle$ is spatially modulated: "phonon density wave"

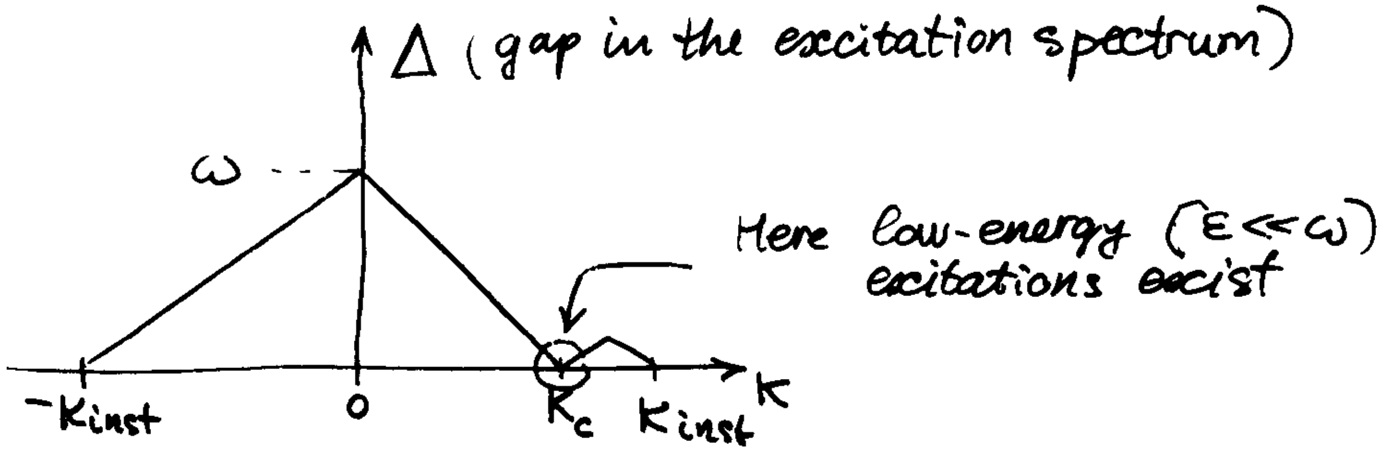
- Quantum effect: vanishes for classic spins or high coordination numbers
$$\frac{K_{inst} - K_c}{K_{inst}} = \frac{1}{1 + zS}$$
(nonmagnetic region shrinks)

- T-inversion symmetry is retained, while translational symmetry is broken.

- Idea of the proof: 1) Find a lower bound: $E_G\{L_\theta\} \geqslant U$

  2) Show, that $E_G\{1,0,1,0\dots\} \equiv U$ for $K_c < K < K_{inst}$

Thermodynamics of the Basic Model



Low energy excitations:

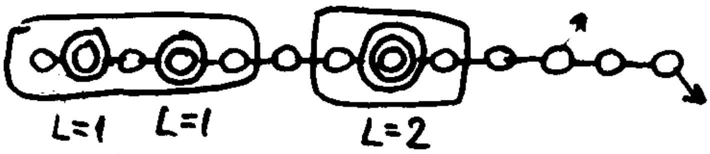
$K < K_c$:

Solitary dimer
$\varepsilon = \Delta_d = 2(K_c - K)$

$K > K_c$:

Solitary free spin
$\varepsilon = \Delta_f = (K - K_c)$

High energy excitations ($\varepsilon \sim \omega$)

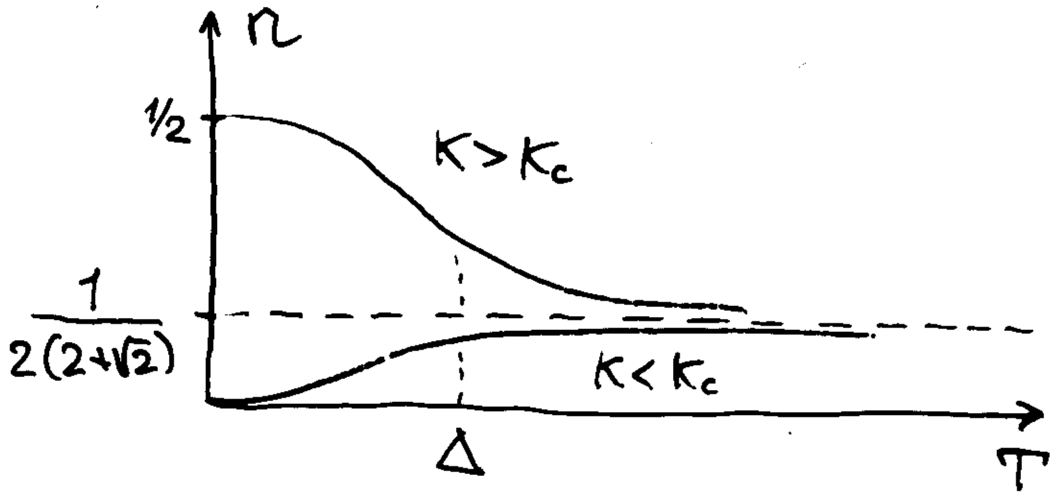


Low energy excitations at $|K - K_c| \ll \omega$:
<u>Partial packings of the chain with singlet dimers without overlap</u>

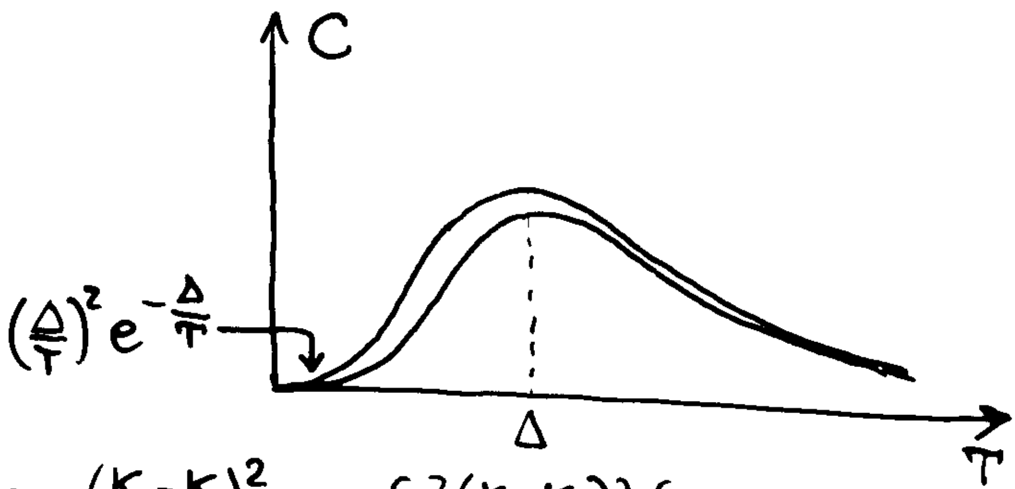
$\Rightarrow$ Classic problem of hard core dimers + entropy of free spins.

In 1-D the partition function can be found explicitly.

Concentration of singlet dimers

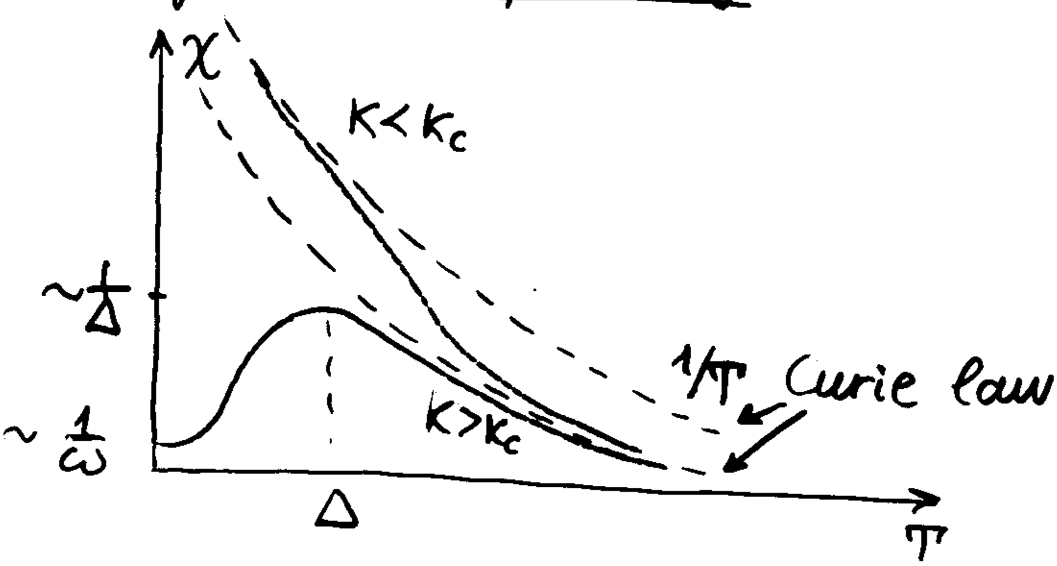


Specific heat



$$C(T) = \left(\frac{K_c - K}{T}\right)^2 \exp\left\{\frac{2(K-K_c)}{T}\right\}\left\{1 + \exp\left\{-\frac{2(K-K_c)}{T}\right\}\right\}^{-3/2}$$

Magnetic susceptibility



Beyond the Basic Model

Small deviations:

- Dispersion of phonons

$$H_{disp} = \frac{U}{2} \sum_{\langle 66' \rangle} (\vec{Q}_6 \vec{Q}_{6'}), \quad U \ll \omega$$

- Spin-spin interactions:

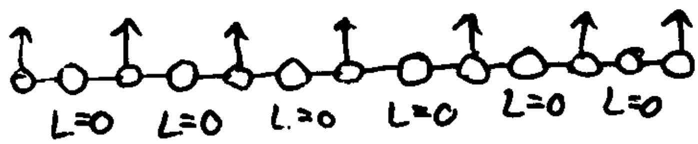
$$H_{mag} = J \sum_{\langle aa' \rangle} (\vec{S}_a \vec{S}_{a'}), \quad J \ll \omega$$

Far below K_c:

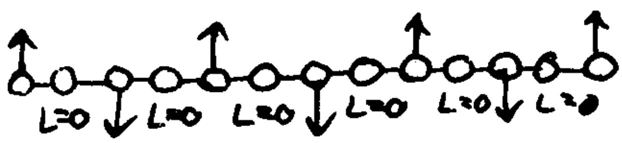
$K < K_c$, $K_c - K \gg U, J$.

In the ground state $\{L_6\} \equiv 0$, spin degeneracy is lifted by H_{mag}:

Ferromagnet for $J<0$



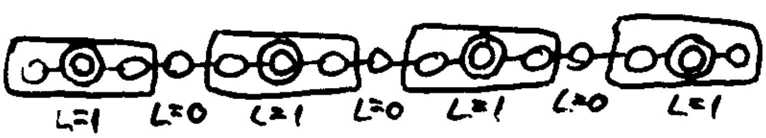
Hulthén singlet for $J>0$ (analog of AF in 3D



Far above K_c:

$K > K_c$, $K - K_c \gg U, J$

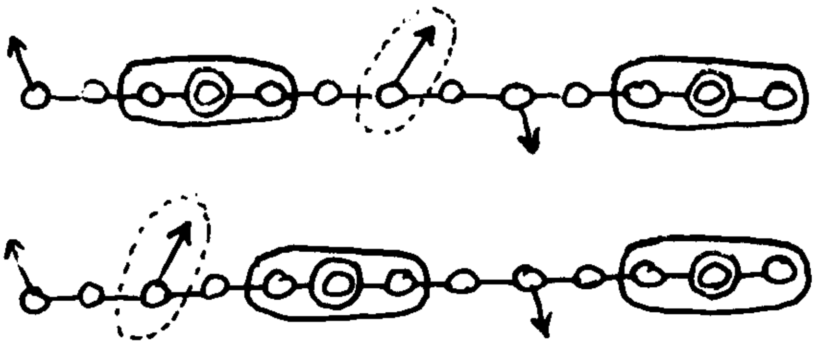
In the ground state $\{L_6\} = (1,0,1,0\ldots)$ the global two-fold degeneracy is not lifted



Close to K_c: Quantum liquid regime

If $|K-K_c| \sim \Delta \lesssim U$: low energy excitations are admixed;
The ground state changes dramatically.

$$H_{disp} \xrightarrow[\text{low-energy subspace}]{\text{projection onto the}} \text{Hopping of dimers}$$



Amplitude of hopping
$\tau \sim U$

Energy loss due to creation of dimer (fre spin): Δ
Energy gain due to its delocalization: t

For $t > \Delta$:

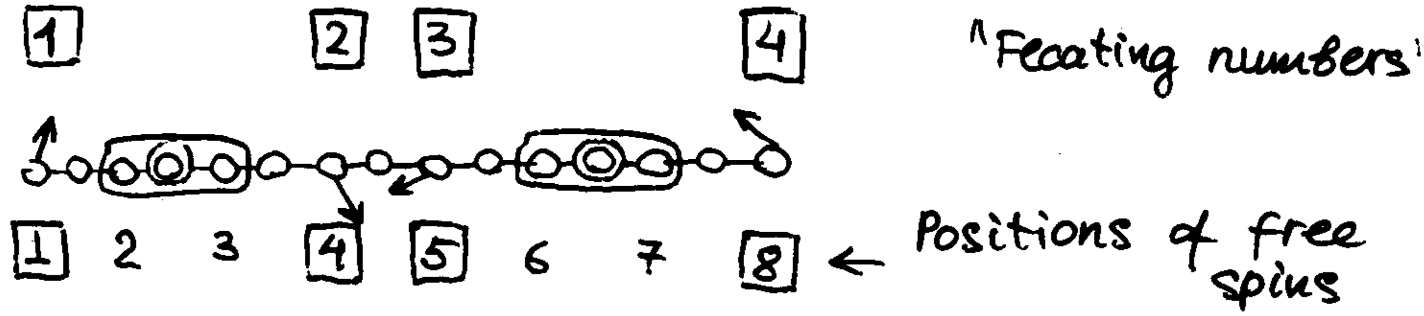
Spontaneous "defect-production" (interaction controlled)

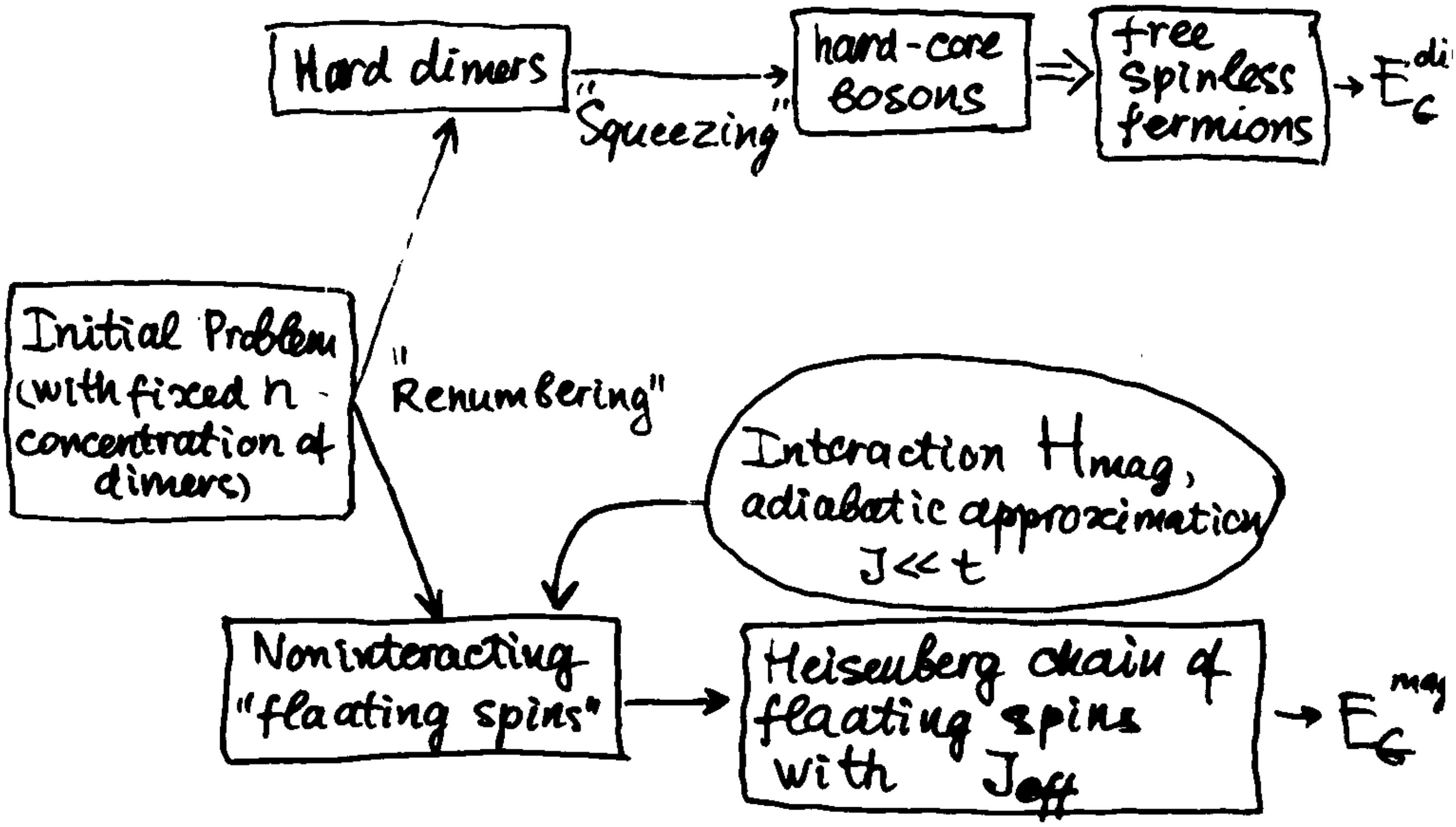
(like in quantum crystals)

Quantum Liquid: coherent mixture of
itinerant singlet dimers
itinerant free spins

In 1-D the problem can be solved exactly (for $J \ll U$)

Exact separation of spin and orbital degrees of freedom: Renumbering transformation





$$E_G^{dim}(n) = 2n(K_c - K) - \frac{2t}{\pi}(1-n)\sin\left(\frac{\pi n}{1-n}\right)$$

$$E_G^{mag}(n) = A(1-2n)\, J_{eff}(n), \quad J_{eff} < J$$

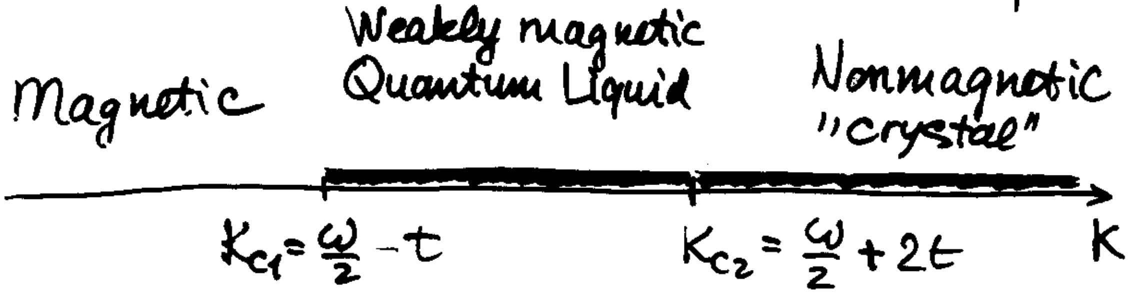
$$E_G(n) = E_G^{dim}(n) + E_G^{mag}(n),$$

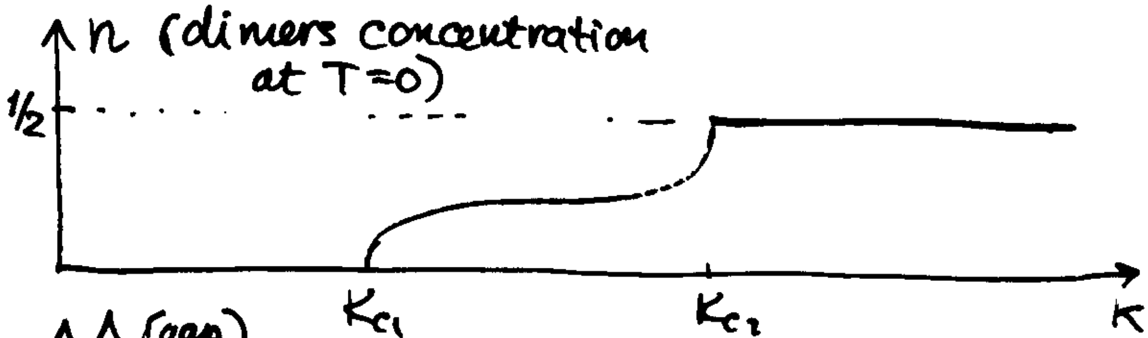
$$E_G^{mag} \ll E_G^{dim}$$

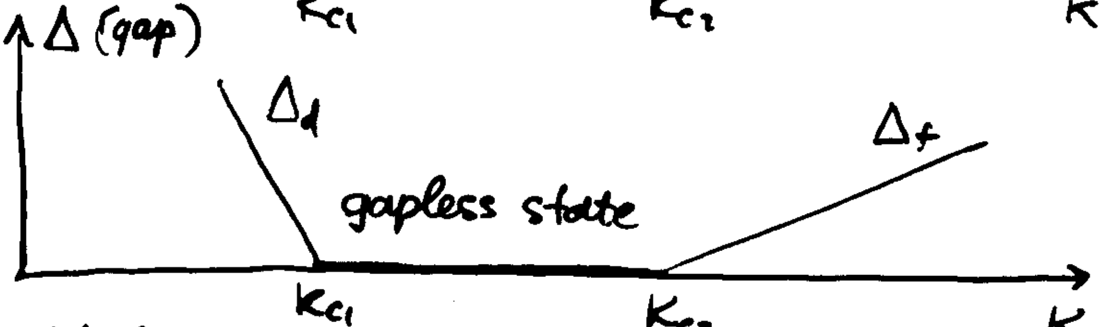
The optimal concentration of dimers n

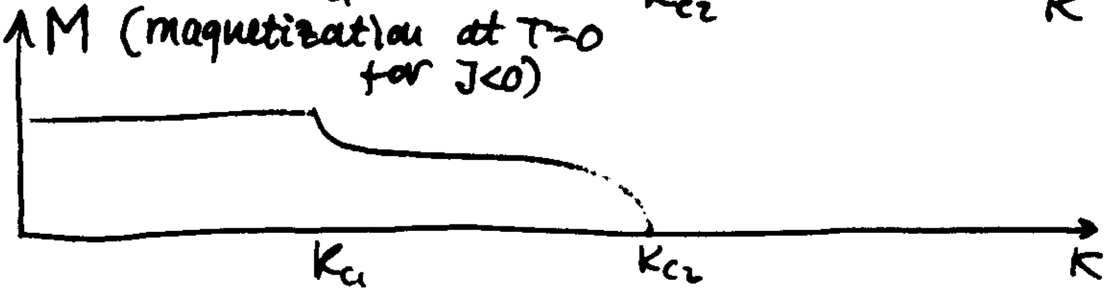
$$\min E_G(n)$$

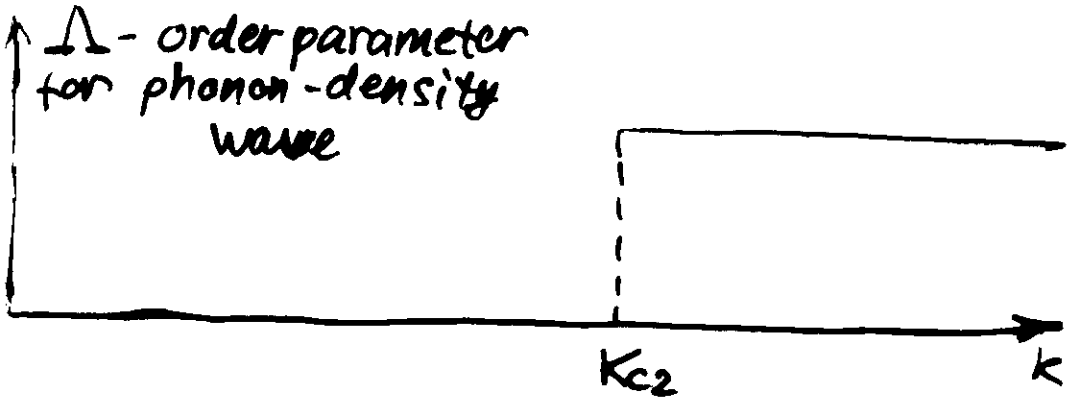
Phase diagram: fragment in the vicinity of K_c:

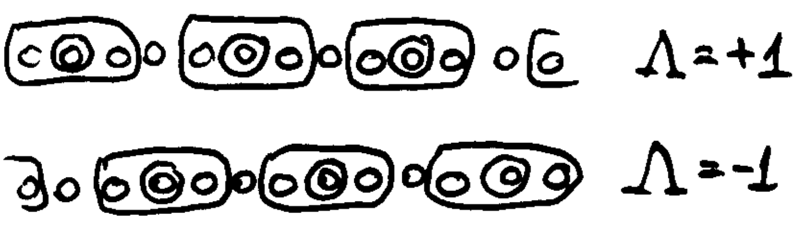








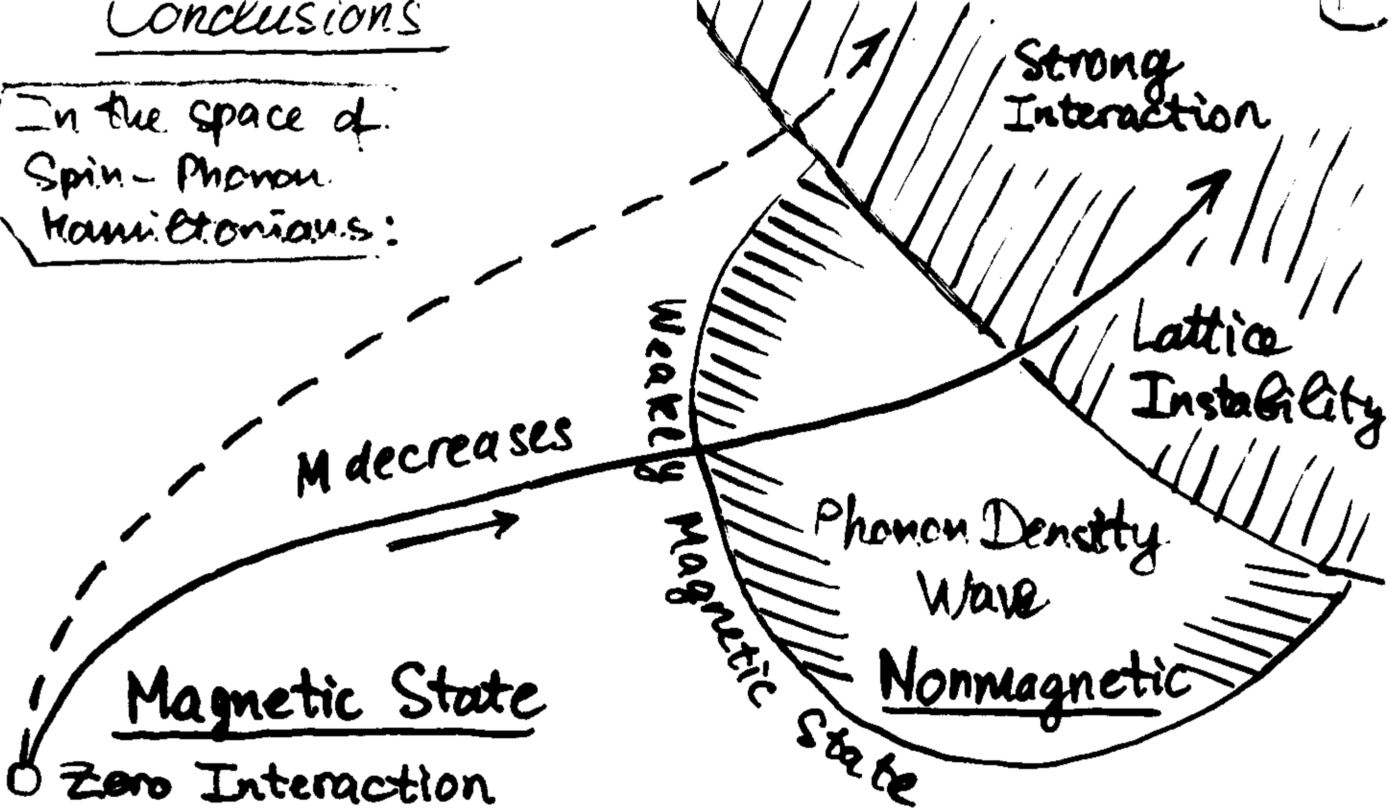




$$\Lambda = \sum_n \langle Q_n^2 \rangle (-1)^n$$

Conclusions

- In the space of Spin-Phonon Hamiltonians:



- Singlet spin-phonon complexes: spins are coupled in groups by the exchange of virtual phonons.

Intracomplex interaction > intercomplex interaction.

- Totally screened (nonmagnetic) state: all spins are in complexes

  Partly screened (weakly magnetic) state: part of spins are in itinerant complexes; other spins are free: quantum liquid

- Open question: properties of the Quantum Liquid in 3D.

  A character of the phase transition?