

Spin-wave calculations for Heisenberg magnets with reduced symmetry

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1.1 Introduction: Magnetism

- Types of magnetism

$$\chi = \frac{\partial \vec{M}}{\partial \vec{H}}$$

- Diamagnetism

response to magnetic field due to Lenz' rule

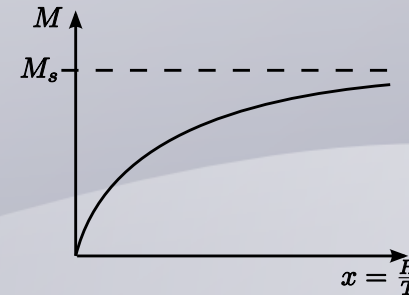
$$\vec{L}|0\rangle = 0 \quad \vec{S}|0\rangle = 0$$

$$\chi = -\frac{e^2}{6m}\mu_0 n r_a^2 Z_a \approx -10^{-4} < 0$$

- Paramagnetism

alignment of magnetic moment in a magnetic field

$$\chi \sim \frac{1}{T} > 0$$



- **Collective magnetism**

correlation effects of spin degrees of freedom

$$\chi \rightarrow \infty \quad (\text{phase transitions})$$

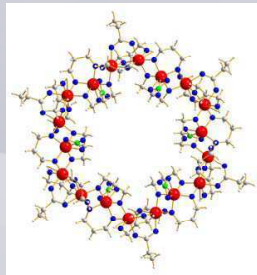


1.2 Introduction: Collective magnetism

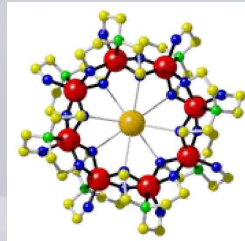
- Itinerant magnetism in metals
magnetization from occupation of states

$$M \sim n_{\uparrow} - n_{\downarrow}$$

- Magnetism on mesoscopic scales



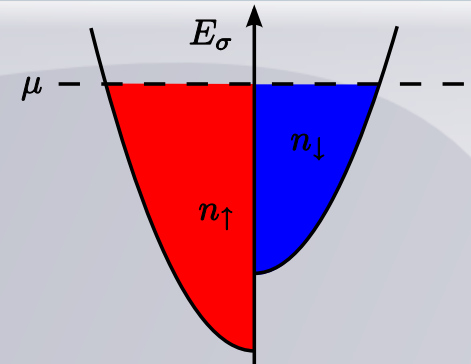
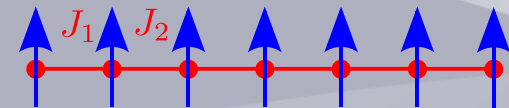
Fe₁₈



CsFe₈

finite numbers of spins:
nevertheless collective
behaviour

method: exact diagonalisation
Waldmann *et al.* PRL ('06)



- Magnetism of localized spins in insulators

$$H = J \vec{S}_1 \cdot \vec{S}_2 \quad \rightarrow \quad H = \frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Heisenberg model

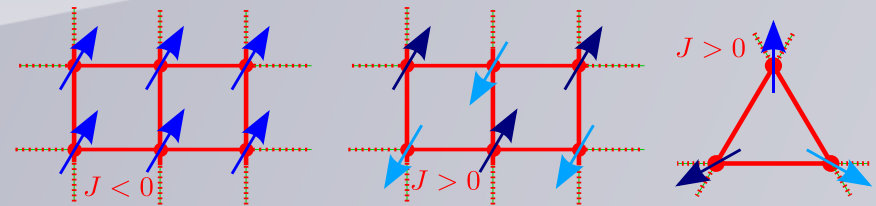
W. Heisenberg Z. Phys. **49**, 619 (1928)



1.3 Introduction: Spin wave theory (method)

- determine classical groundstate

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



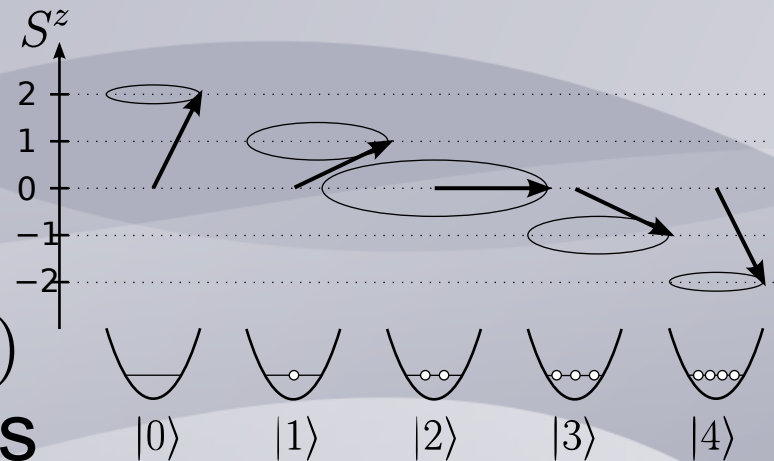
- expand in terms of bosons

- Holstein-Primakoff transformation
- Expansion in powers of $1/S$
exact for $S \rightarrow \infty$, but $S = \mathcal{O}(1)$

Holstein, Primakoff
Phys. Rev. ('40)

- Interacting theory of bosons

- Methods of quantum mechanics
- Theory of many particle systems



$$H = \sum_{\vec{k}} E_{\vec{k}} b_{\vec{k}}^{\dagger} b_{\vec{k}} + \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} \Gamma^3(\vec{k}_1, \vec{k}_2, \vec{k}_3) b_{\vec{k}_1}^{\dagger} b_{\vec{k}_2} b_{\vec{k}_3} + \sum_{1,2,3,4} \Gamma^4(1, 2; 3, 4) b_1^{\dagger} b_2^{\dagger} b_3 b_4 + \dots$$



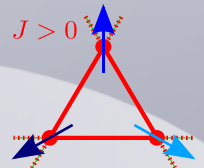
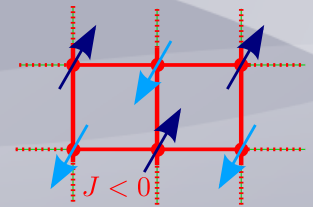
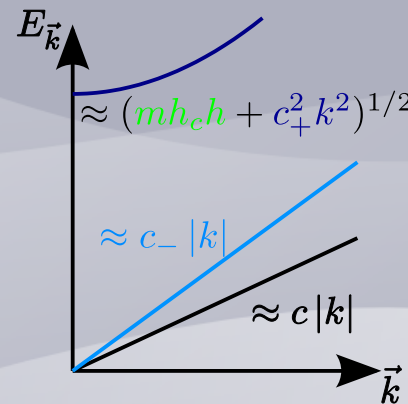
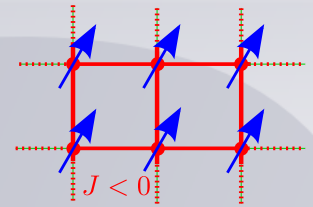
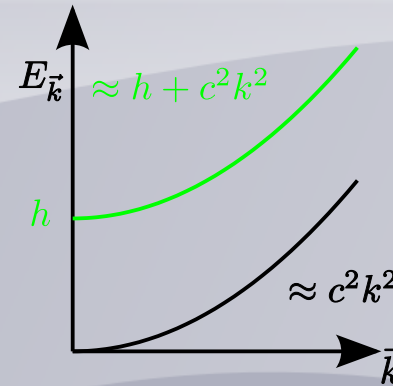
1.4 Introduction: Spin waves (general results)

- Ferromagnet
(exchange interaction only)
 - Quadratic excitation spectrum
 - Vanishing interaction at $k=0$

$$\Gamma^4 \sim -(\vec{k}_1 \cdot \vec{k}_2 + \vec{k}_3 \cdot \vec{k}_4)$$

- Antiferromagnet
 - Linear spectrum
(Goldstone mode)
 - Two modes in magnetic field
(2 sublattices)
 - Divergent interaction vertices

$$\Gamma^4 \sim \sqrt{\frac{|\vec{k}_1||\vec{k}_2|}{|\vec{k}_3||\vec{k}_4|}} \left(1 \pm \frac{\vec{k}_1 \cdot \vec{k}_2}{|\vec{k}_1||\vec{k}_2|} \right)$$



Hasselmann, Kopietz, EPL ('06)
 Chernychev, Zhitomirsky, PRB ('09)
 Veillette *et al.* PRB ('05)
 AK, *et al.* PRB ('08)

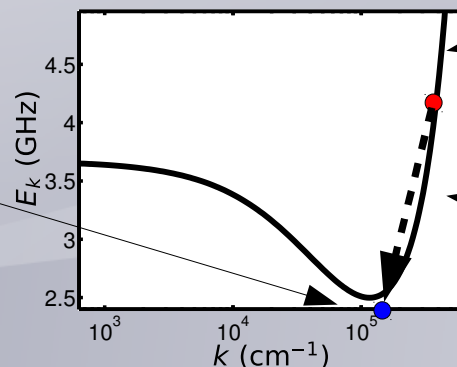


2.1 Model system 1: Thin-film ferromagnet

- Motivation: Experiments on YIG (yttrium iron garnet) films
 - Excitation and detection of spin waves with high energy resolution (parametric pumping, Brillouin light scattering spectroscopy)
 - Low spin-wave damping in YIG
 - Good experimental control

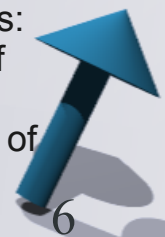
Observation of the occupation number using microwave antennas or Brillouin Light Scattering (BLS)
Sandweg, *et al.*
Rev. Sci. Instrum. ('10)

Condensation of magnons at room temperature!
Demokritov *et al.* Nature ('06)



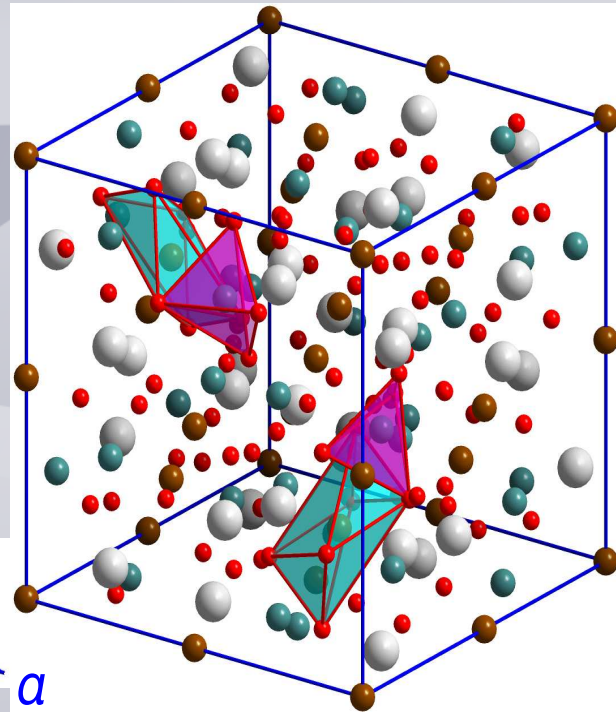
Parametric pumping of magnons at high k-vectors creates magnetic excitations

Open questions:
Time evolution of magnons:
Non-equilibrium physics of interacting quasiparticles?
Coupling to other degrees of freedom, thermalization?
Kloss, Kopietz PRB ('11)



2.2 Model system 1: Microscopic model

Crystal structure of YIG



16a: Fe

24c: Y

24d: Fe

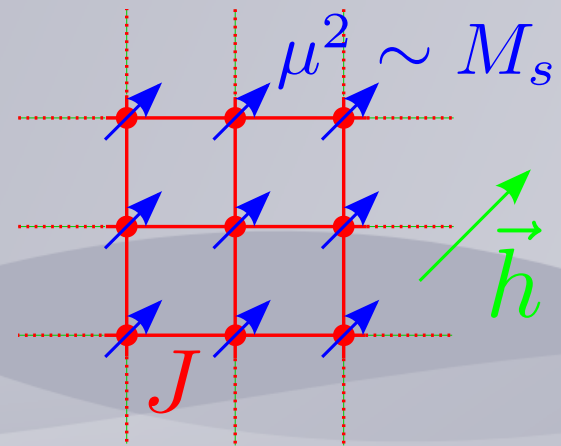
96h: O

space group: **1a3d**
 Y: 24(c) white
 Fe: 24(d) green
 Fe: 16(a) brown
 O: 96(h) red

Gilleo, Geller Phys. Rev. ('58)

Magnetic system:
 40 magnetic ions in
 elementary cell
 40 magnetic bands

Microscopic Hamiltonian



reduced
symmetry

quantum spin **S**
ferromagnet

Zeeman
term

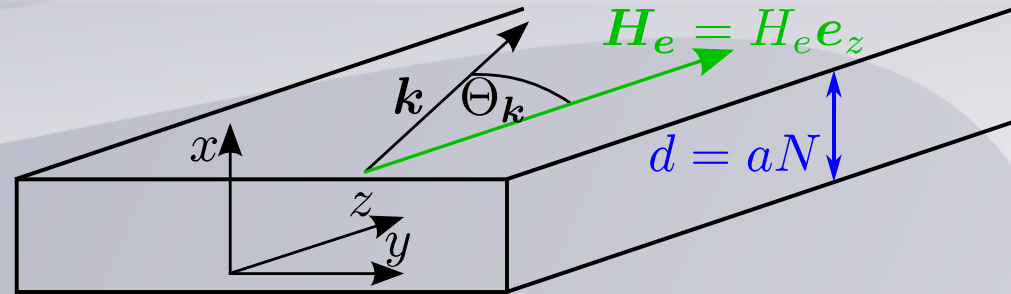
dipole-dipole
interactions

$$\hat{H}_{\text{mag}} = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z - \frac{1}{2} \sum_i \sum_{j \neq i} \frac{\mu^2}{|\mathbf{r}_{ij}|^3} [3(\mathbf{S}_i \cdot \hat{\mathbf{r}}_{ij})(\mathbf{S}_j \cdot \hat{\mathbf{r}}_{ij}) - \mathbf{S}_i \cdot \mathbf{S}_j]$$



2.3 Model system 1: Linear spin-wave theory

- Geometry (thin film)



- Numerical approach

- Ewald summation technique
- Diagonalization of $2N \times 2N$ matrix

$$H_2 = \begin{pmatrix} A_{\vec{k}} & B_{\vec{k}} \\ B_{-\vec{k}}^* & -A_{-\vec{k}}^T \end{pmatrix}$$

- Analytic approaches

- Approximation for lowest mode
- Bogoliubov transformation

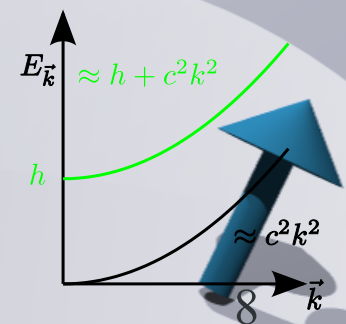
$$E_{\vec{k}} = \sqrt{[h + \rho_{\text{ex}} \vec{k}^2 + \Delta(1 - f_{\vec{k}}) \sin^2 \Theta_{\vec{k}}][h + \rho_{\text{ex}} \vec{k}^2 + \Delta f_{\vec{k}}]}$$

$$\Delta = 4\pi\mu M_S$$

- No dipolar interaction: known result

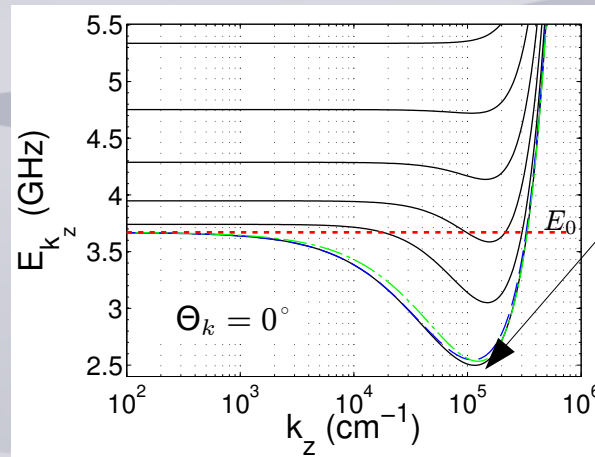
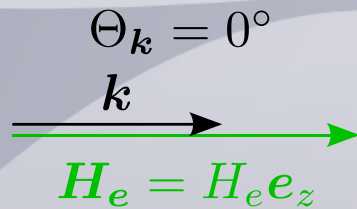
$$E_{\vec{k}} = h + \rho_{\text{ex}} \vec{k}^2 \quad \Delta = 0$$

structure factor

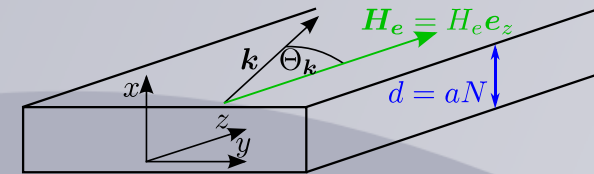


2.4 Model system 1: Results for spectra

- Parallel mode



Minimum for BEC
Demokritov *et al.*
Nature ('06)



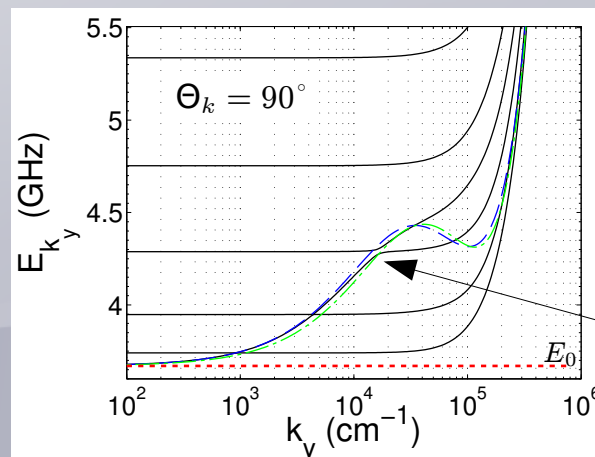
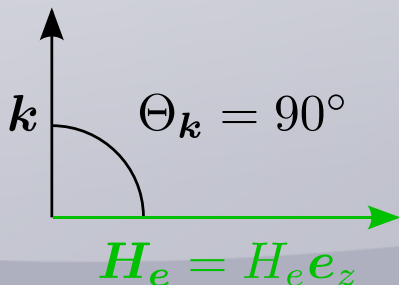
$$d = 400a \approx 0.5 \mu\text{m}$$

$$N = 400$$

$$H_e = 700 \text{ Oe}$$

$$E_0 = \sqrt{h(h + 4\pi\mu M_s)}$$

- Perpendicular mode



Hybridization:
surface mode



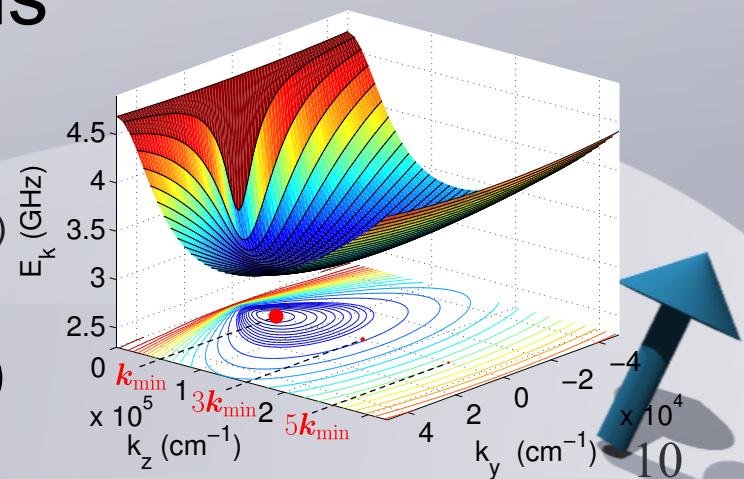
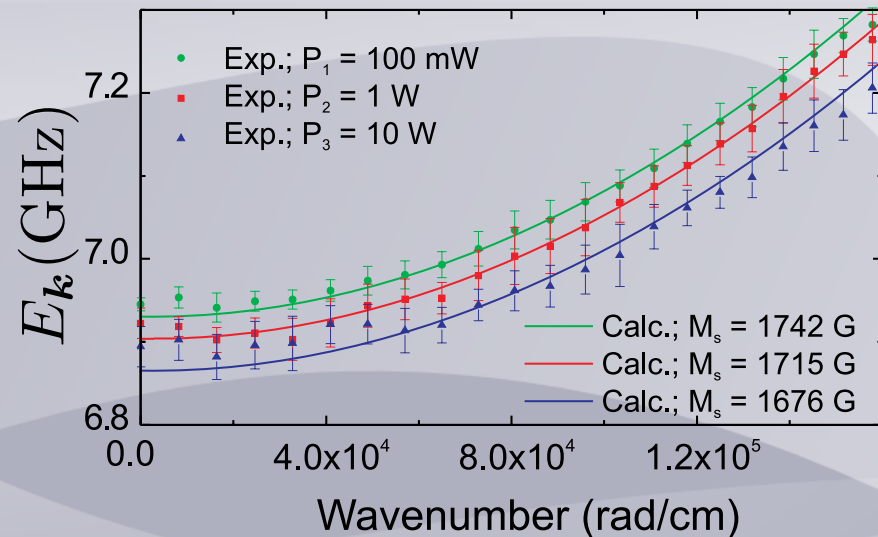
2.5: Model system 1: Comparison to experiments

- Excitation and detection of spinwaves using Brillouin light scattering spectroscopy (BLS)

$$\Theta_{\vec{k}} = 90^\circ$$

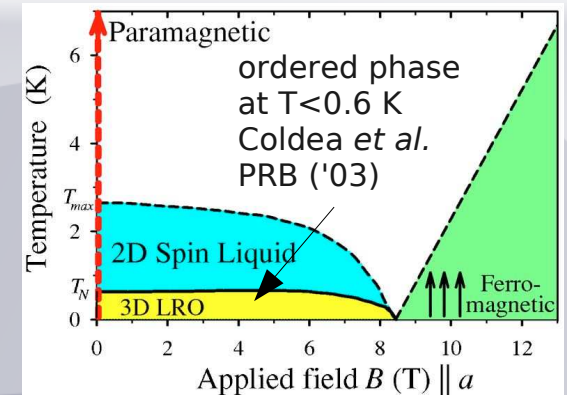
- Outlook, future investigations
 - Condensation of magnons (nonequilibrium, finite momentum)
 - Interactions (magnon-magnon, magnon-phonon)

Hick *et al.* EPJB ('10)



Triangular antiferromagnet

- Exactly **known microscopic model** for the frustrated antiferromagnet Cs_2CuCl_4



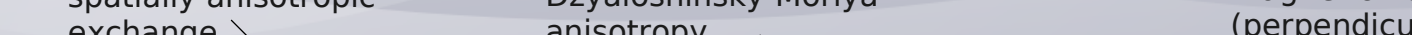
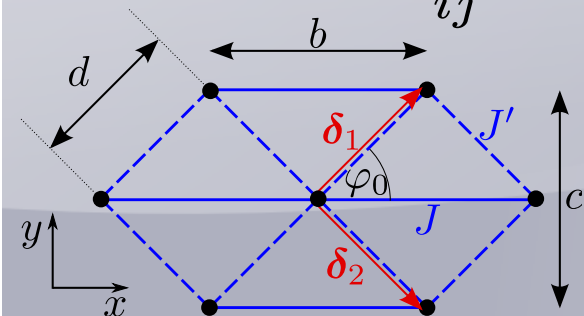


Diagram illustrating the spin Hamiltonian $\hat{H}_{\text{spin}}$ with annotations for each term:

- spatially anisotropic exchange**: points to J_{ij}
- Dzyaloshinsky-Moriya anisotropy**: points to $\mathbf{D}_{ij}$
- magnetic field (perpendicular to plane)**: points to $\mathbf{h}$

$$\hat{H}_{\text{spin}} = \frac{1}{2} \sum_{ij} [J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)] - \sum_i \mathbf{h} \cdot \mathbf{S}_i,$$



$$J_{ij} = J(\mathbf{R}_i - \mathbf{R}_j) = \begin{cases} J & \text{if } \mathbf{R}_i - \mathbf{R}_j = \pm(\delta_1 + \delta_2) \\ J' & \text{if } \mathbf{R}_i - \mathbf{R}_j = \pm\delta_1 \text{ or } \pm\delta_2 \end{cases}$$

$$D_{ij} = \pm D e_z$$

$J=0.37$ meV
 $J'=0.13$ meV
 $D=0.02$ meV

Coldea *et al.* PRL ('02)

3.2 Model system 2: Spin-wave approach

- Classical groundstate:
“cone state”

Veillette *et al.* PRB ('05)

- Spin-wave spectra

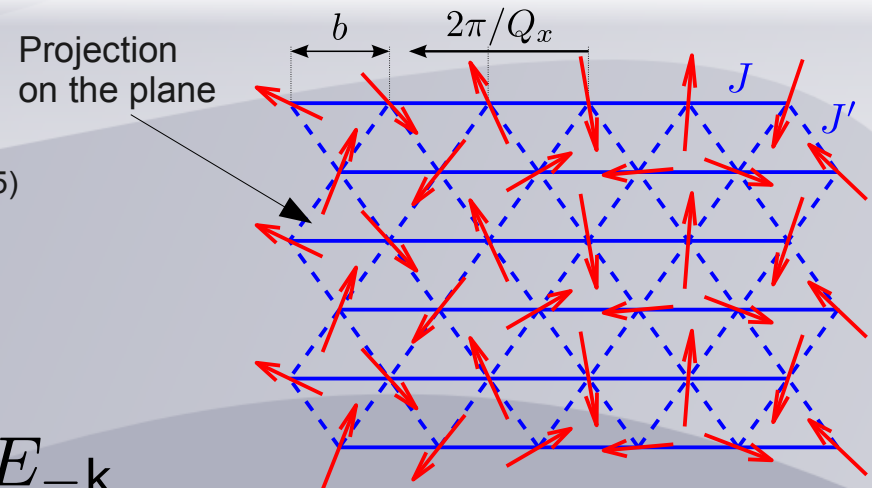
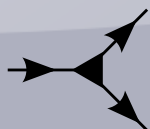
$$E_k = \sqrt{(A_k^+)^2 - B_k^2} + A_k^- \neq E_{-k}$$

symmetric with respect to k

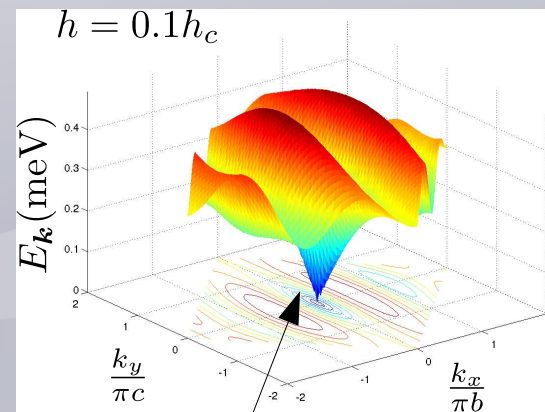
antisymmetric, but $\propto k^3$
(Dzyaloshinsky-Moria anisotropy)

- Interactions
 - Large for finite field

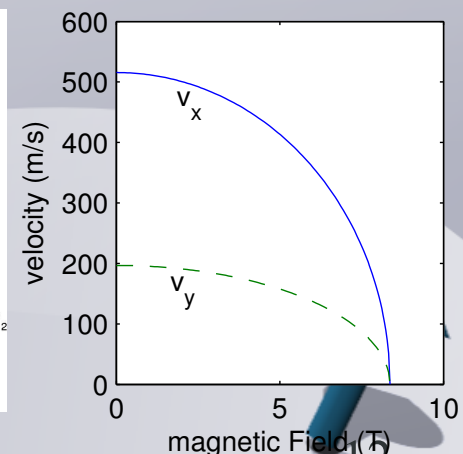
$$\Gamma_3^{b^\dagger b^\dagger b}(k_1, k_2; k_3) \approx -\frac{\hbar}{\hbar_c} \sqrt{1 - \left(\frac{\hbar}{\hbar_c}\right)^2} \frac{\sqrt{2S}}{i} \frac{\hbar_c}{S}$$



$$E_k = \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2} + \mathcal{O}(k^3)$$



Goldstone mode: U(1) symmetry

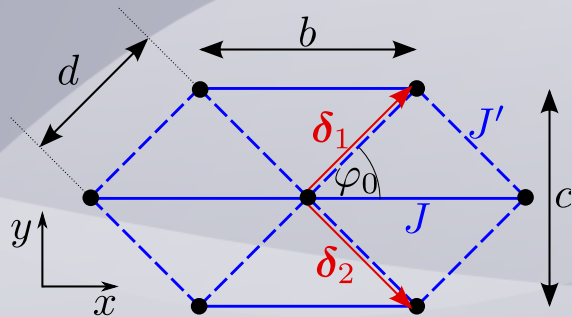


3.3 Model system 2: Coupling to lattice vibrations

- Include **lattice vibrations**

$$H = \frac{1}{2} \sum_{ij} [J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)] - \sum_i \mathbf{h} \cdot \mathbf{S}_i$$

← exchange
← DM anisotropy



$$+ \sum_{\mathbf{k}\lambda} \left[\frac{P_{-\mathbf{k}\lambda} P_{\mathbf{k}\lambda}}{2M} + \frac{M}{2} \omega_{\mathbf{k}\lambda}^2 X_{-\mathbf{k}\lambda} X_{\mathbf{k}\lambda} \right]$$

$\omega_{\mathbf{k}\lambda} = c_\lambda(\hat{\mathbf{k}})|\mathbf{k}|$
← phonon dispersion (acoustic)

- Spin-phonon coupling** via expansion of exchange integrals

$$J_{ij} = J(\mathbf{R}_{ij}) + (\mathbf{X}_{ij} \cdot \nabla_{\mathbf{R}}) J(\mathbf{r})|_{\mathbf{r}=\mathbf{r}_{ij}} + \dots = J(\mathbf{R}_{ij}) + \mathbf{X}_{ij} \cdot \mathbf{J}_{ij}^{(1)} + \dots$$

← bare exchange
← magnon phonon coupling

$$D_{ij} \approx D(\mathbf{R}_{ij})$$



3.4 Model system 2: Calculation of observables

- Shift of the **phonon velocity**

- Integrate out magnetic degrees of freedom

$$e^{-S_{\text{eff}}^{\text{2pho}}[\mathbf{X}]} = \int \mathcal{D}[\boldsymbol{\beta}, \bar{\boldsymbol{\beta}}] e^{-S^{\text{2pho}}[\mathbf{X}] - S_{\text{2mag}}[\bar{\boldsymbol{\beta}}, \boldsymbol{\beta}] - S_{\text{1pho}}^{\text{1pho}}[\mathbf{X}, \bar{\boldsymbol{\beta}}, \boldsymbol{\beta}]}$$

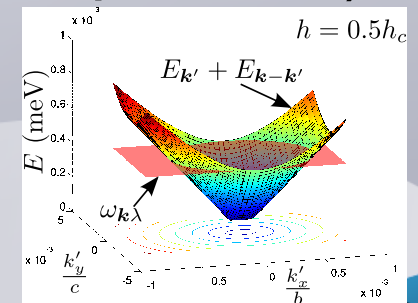
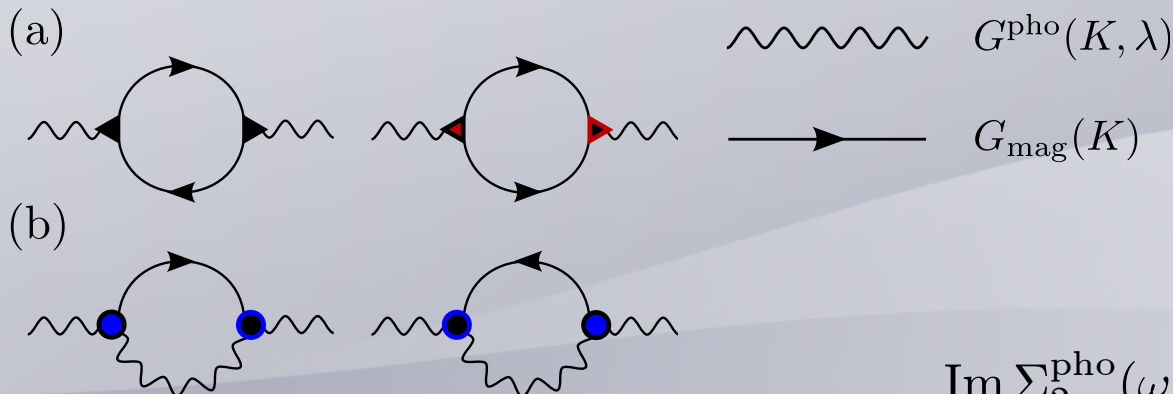
$$\frac{(\Delta c_{\lambda})_{\text{tot}}}{c_{\lambda}} = \lim_{|\mathbf{k}| \rightarrow 0} \left(\sqrt{1 - \frac{\Sigma_0^{\text{pho}}(\mathbf{k}, \lambda)}{\omega_{\mathbf{k}\lambda}^2}} - 1 + \frac{|\Gamma_{\mathbf{k}}^{X\beta} \cdot \mathbf{e}_{\mathbf{k}\lambda}|^2}{2M\omega_{\mathbf{k}\lambda}^3} \right)$$

Two contributions:

1. Classical spin background
2. Hybridization to magnetoelastic waves

- Ultrasound **attenuation rate**

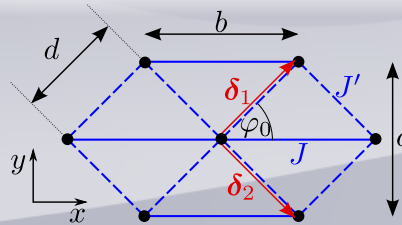
- Diagrammatic perturbation theory (1/S expansion)



$$\gamma_{\mathbf{k}\lambda} = - \frac{\text{Im} \Sigma_2^{\text{pho}}(\omega_{\mathbf{k}\lambda} + i0^+, \mathbf{k}, \lambda)}{2\omega_{\mathbf{k}\lambda}}$$

3.5 Model system 2: Comparison to experiments

- Model



$$J(x) = J(b)e^{-\kappa(x-b)/b}$$

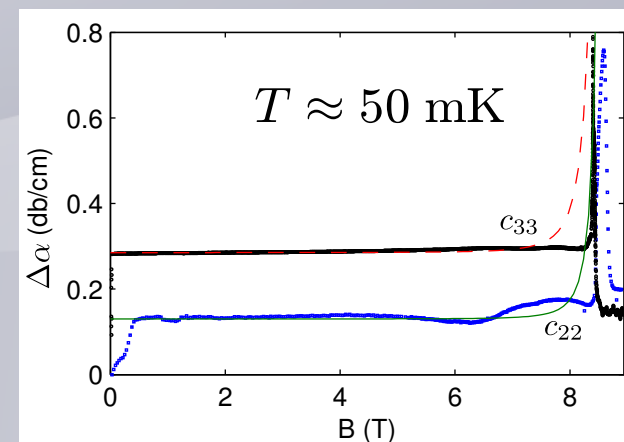
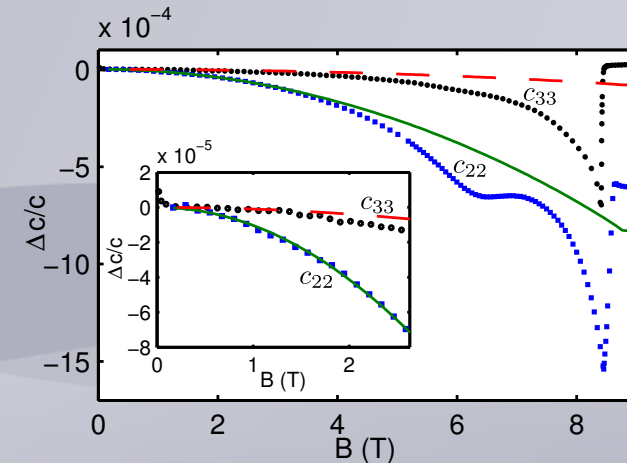
$$J'(r) = J'(d)e^{-\kappa'(r-d)/d}$$

- Shift of ultrasound velocity for c_{22} mode (P. T. Cong):

- Fix parameters: $\kappa \approx 15$ $\kappa' \approx 51$
- Project result for c_{33} mode without adjustable parameters

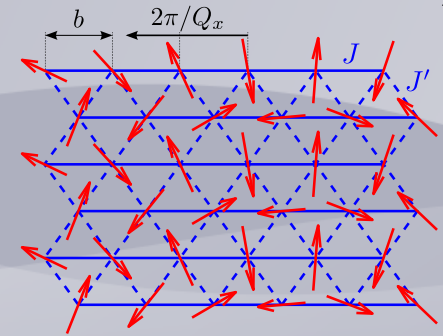
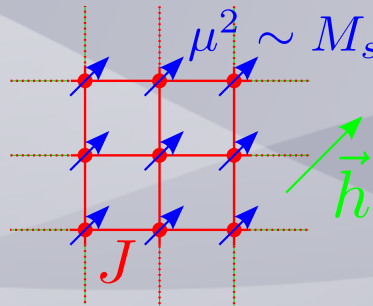
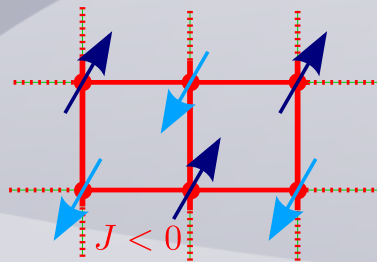
- Attenuation rate calculate from parameters

$$\gamma_{k\lambda} \approx \frac{\pi^2}{64} \left(\frac{k^2}{2M} \right) \left(\frac{S^2 c_\lambda^2 k^2}{V_{BZ} v_x v_y} \right) \frac{[\mathbf{f}_1^{X\beta}(\hat{\mathbf{k}}) \cdot \mathbf{e}_{k\lambda}]^2}{(1 - h/h_c)^2}$$



4 Summary

- Theoretical investigations on **Heisenberg magnets with reduced symmetry**
 - 3 different model systems (2 presented in detail)



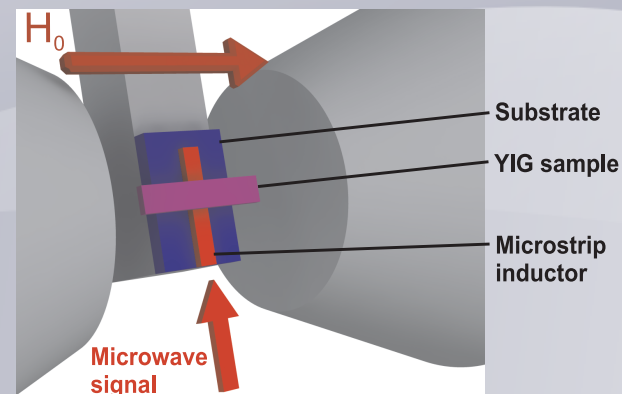
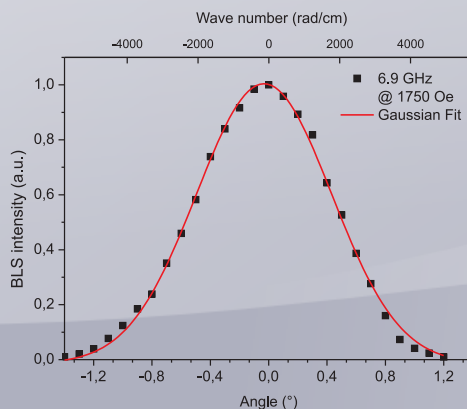
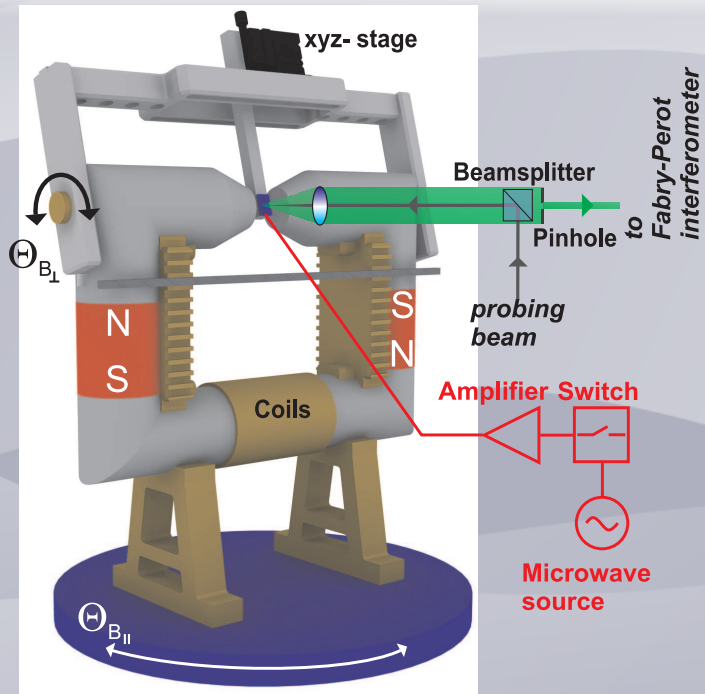
- Application and further **development of concepts** using the spin-wave approach
- Connection to recent experimental research and comparison of corresponding results



5.1 Experimental details

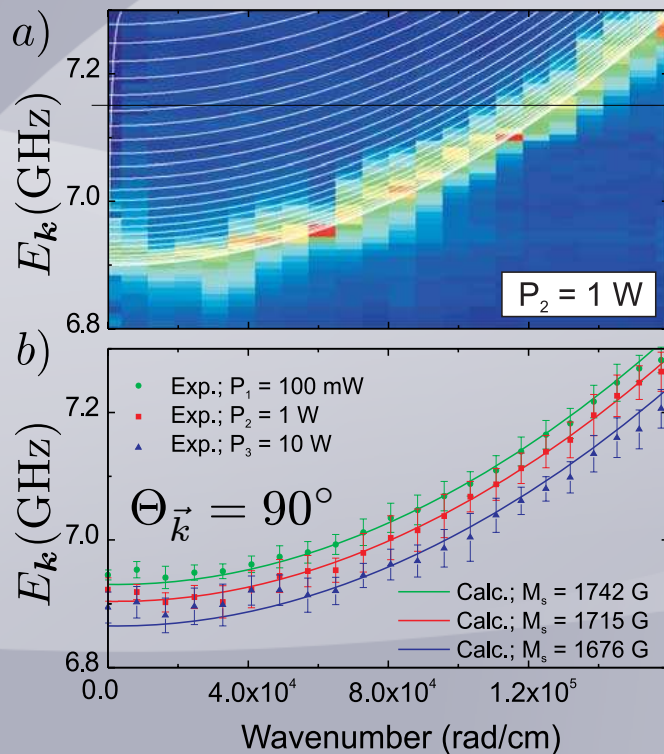
BLS spectroscopy

- Wavevector resolved BLS setup (C. Sandweg, TU Kaiserslautern)
- large wave vector range
- high resolution



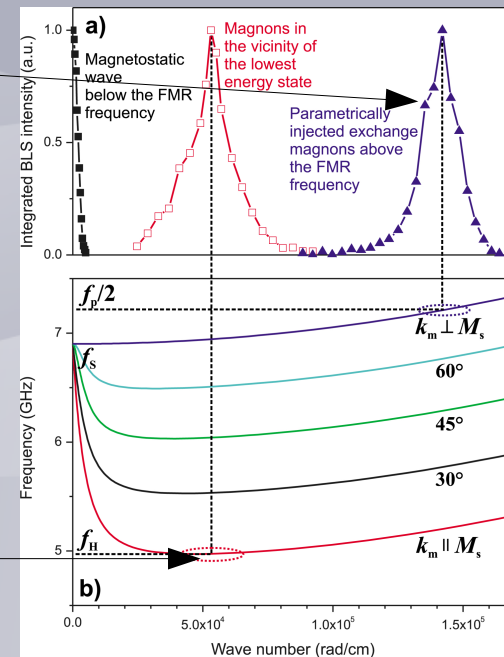
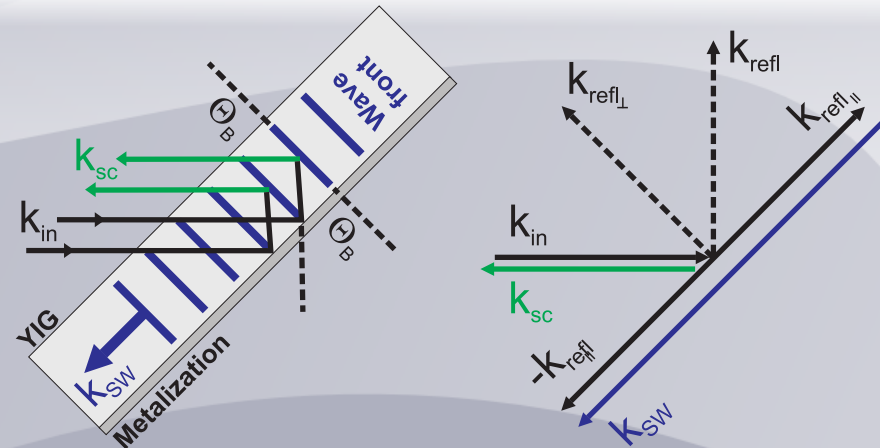
5.2: Experimental Details BLS spectroscopy

- Scattering of light on grating created from spin waves



cut along
line

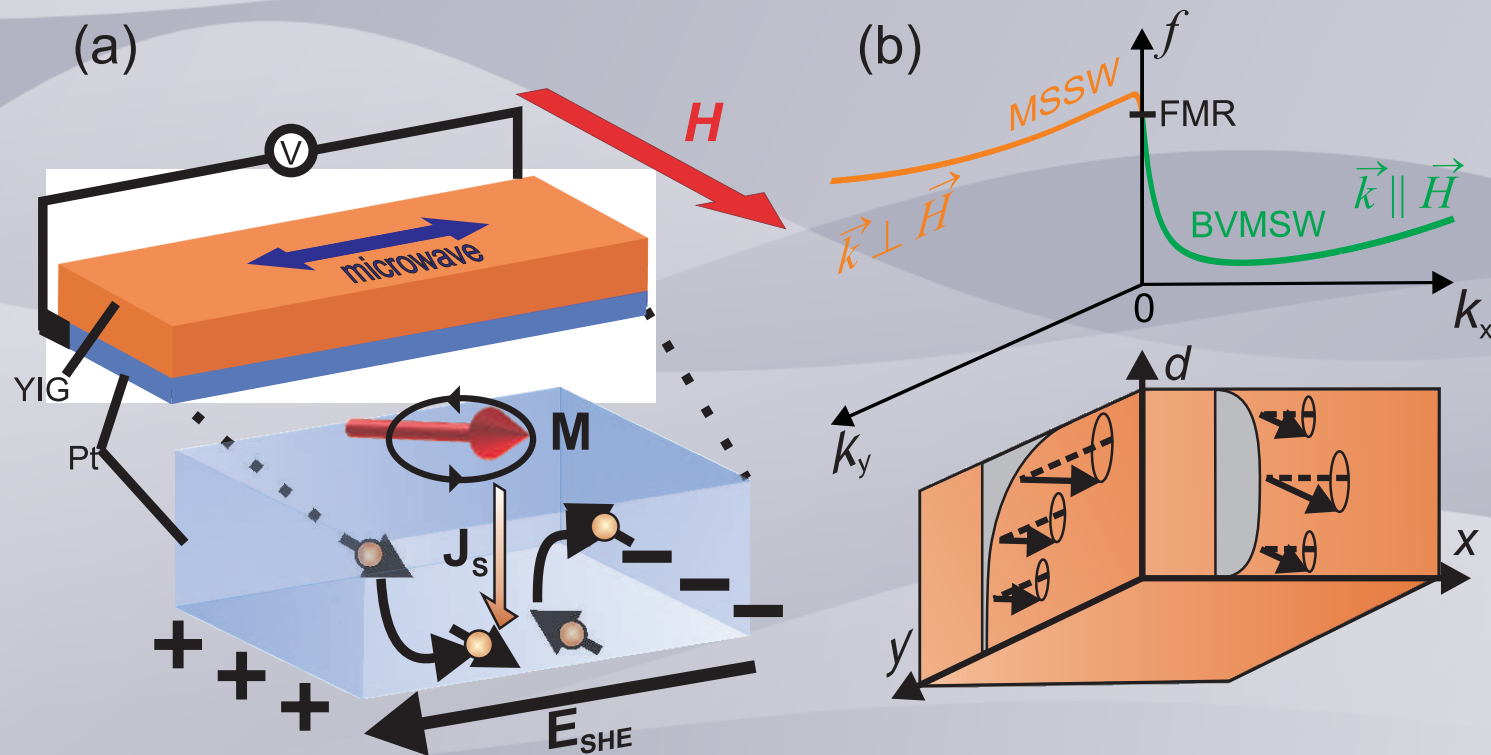
wavenumber
from geometry
energy from
interferometer



5.3 Experimental details

Techniques: Thin-film magnets

- Inverse spin-hall effect (ISHE): spin polarized current



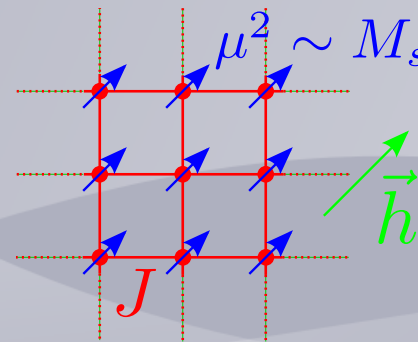
5.4 Experimental details

Material parameters for YIG

- Heisenberg magnet with dipole-dipole interactions

$$\hat{H}_{\text{mag}} = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z$$

$$- \frac{1}{2} \sum_i \sum_{j \neq i} \frac{\mu^2}{|\mathbf{r}_{ij}|^3} [3(\mathbf{S}_i \cdot \hat{\mathbf{r}}_{ij})(\mathbf{S}_j \cdot \hat{\mathbf{r}}_{ij}) - \mathbf{S}_i \cdot \mathbf{S}_j]$$



material
parameters

$$a = 12.376 \text{ \AA}$$

Gilleo *et al.* '58

$$4\pi M_s = 1750 \text{ G}$$

Tittmann '73

$$\frac{\rho_{\text{ex}}}{\mu} = 5.17 \cdot 10^{-13} \text{ Oe m}^2$$

Cherepanov *et al.* '93

alternatively

$$J = 1.29 \text{ K}$$

$$S = 14.2 \quad \mu = 2\mu_B$$

Tupitsyn *et al.* '08

Crystal structure:

space group: **1a3d**

Y: 24(c) white

Fe: 24(d) green

Fe: 16(a) brown

O: 96(h) red

Gilleo *et al.* '58

Magnetic system:

40 magnetic ions in elementary cell

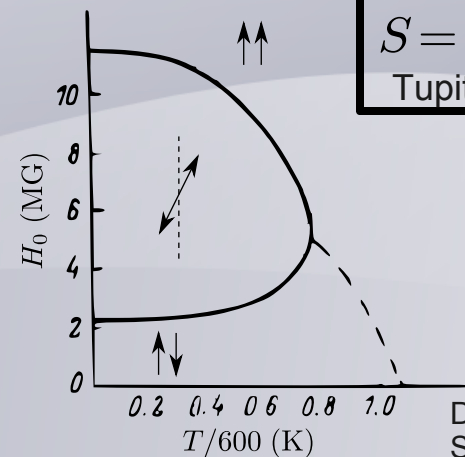
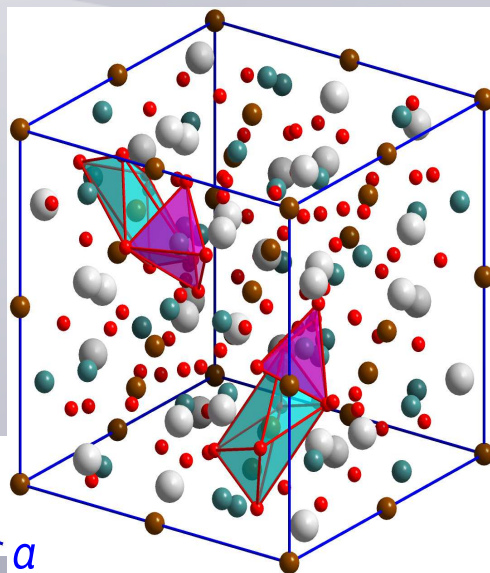
40 magnetic bands

Elastic system:

160 atoms in

elementary cell

3x160 phonon bands



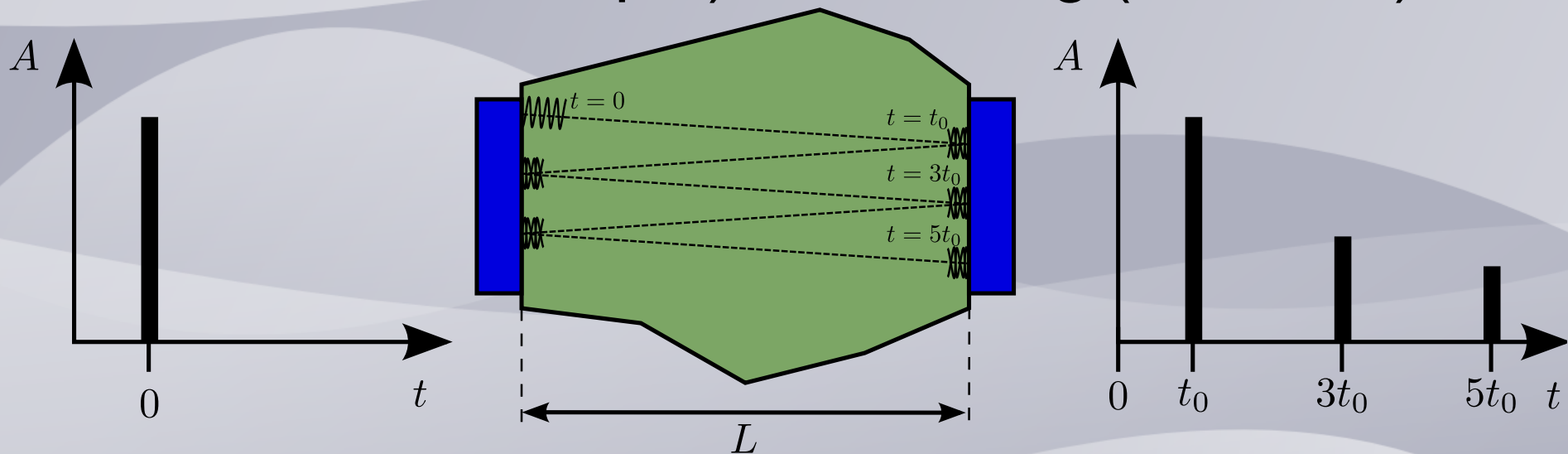
Druzinin *et al.* '20
Sov. Phys. Solid. ('81)



5.5 Experimental details

Ultrasonic technique

- pulse echo method (phase-sensitive detection technique), P. T. Cong (Uni FFM)



- sound velocity $c_\lambda = L/t_0$
- change of sound velocity
- (relative) attenuation rate

$$\frac{df}{f} = \frac{dc_\lambda}{c_\lambda}$$

$$\Delta\alpha \propto \frac{1}{L} \ln(A_1/A_0)$$

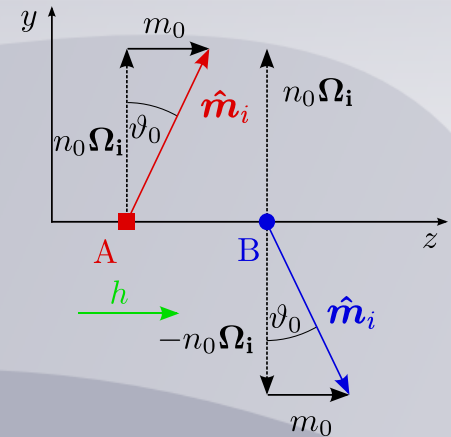
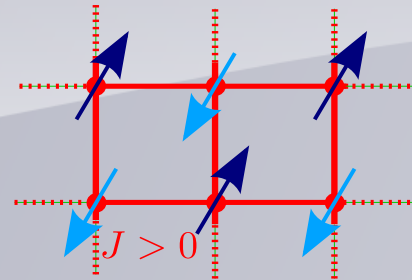


6.1 Theoretical details

QAF in a magnetic field

- model Hamiltonian

$$\hat{H} = \frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z$$



- spin-wave modes

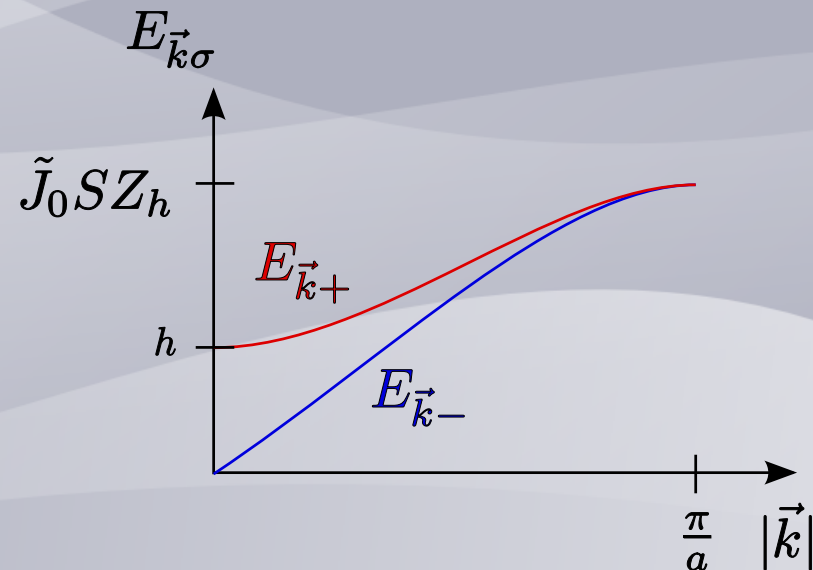
$$E_{\vec{k}+}^2 = h^2 + c_+^2 \vec{k}^2,$$

$$E_{\vec{k}-}^2 = c_-^2 \vec{k}^2,$$

- spin-wave velocities

$$c_+^2 = c_0^2 \left(1 - \frac{3}{\Delta_0^2} h^2\right)$$

$$c_-^2 = c_0^2 \left(1 - \frac{1}{\Delta_0^2} h^2\right)$$



6.2 Theoretical details

QAF in a magnetic field

- Hermitian parametrization (compare harmonic oscillator)

$$[\hat{X}_{\vec{k}\sigma}, \hat{P}_{\vec{k}'\sigma'}] = i\delta_{\vec{k}, -\vec{k}'}\delta_{\sigma, \sigma'}$$

$$\hat{\Psi}_{\vec{k}\sigma} = p_{\sigma} \left[\sqrt{\frac{\nu_{\vec{k}\sigma}}{2}} \hat{X}_{\vec{k}\sigma} + \frac{i}{\sqrt{2\nu_{\vec{k}\sigma}}} \hat{P}_{\vec{k}\sigma} \right]$$

- physical meaning for $k \ll 1$

$\hat{P}_{\vec{k}\sigma}$: uniform spin fluctuations

$\hat{X}_{\vec{k}\sigma}$: staggered spin fluctuations

- effective action

$$S_{\text{eff}}[X_{\sigma}] = S_0 + \frac{\beta}{2} \sum_{K\sigma} \frac{E_{K\sigma}^2 + \omega^2}{\Delta_{K\sigma}} X_{-K\sigma} X_{K\sigma}$$

$$+ \beta \sqrt{\frac{2}{N}} \sum_{K_1 K_2 K_3} \delta_{K_1 + K_2 + K_3, 0} \left[\frac{1}{3!} \Gamma_{---}^{(3)}(K_1, K_2, K_3) X_{K_1-} X_{K_2-} X_{K_3-} \right.$$

$$\left. + \frac{1}{3!} \Gamma_{-++}^{(3)}(K_1; K_2, K_3) X_{K_1-} X_{K_2+} X_{K_3+} \right]$$

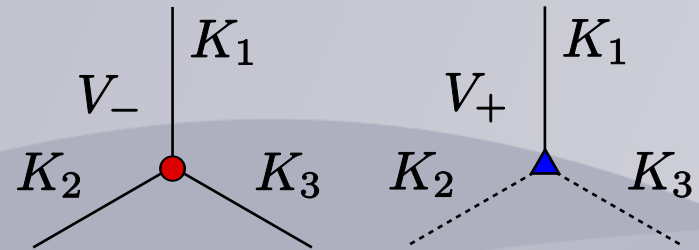


6.3 Theoretical details QAF in a magnetic field

- diagrammatic perturbation theory

$$S_{\text{eff}}^{\text{int}}[X_{\sigma}] = \beta \sqrt{\frac{2}{N}} \sum \left[\frac{1}{3!} V_{-}^{(3)} X_{-} X_{-} X_{-} + \frac{1}{2!} V_{+}^{(3)} X_{-} X_{+} X_{+} \right]$$

$$G_{\sigma}(K) = \frac{\Delta_{k\sigma}}{E_{k\sigma}^2 + \omega^2}$$



- perturbation theory: 1/S corrections to self energy

$$\Sigma_{-} = -\frac{1}{2} \left[\text{diagram 1} + \text{diagram 2} + \text{diagram 3} \right]$$

$$\Sigma_{+} = -\frac{1}{2} \left[\text{diagram 4} + \text{diagram 5} + \text{diagram 6} \right]$$

The diagrams in the brackets represent various self-energy corrections. In the Σ_{-} row, the third diagram is crossed out with a red line. In the Σ_{+} row, the second and third diagrams are crossed out with red lines.

no frequency
dependence,
negligible



6.4 Theoretical details QAF in a magnetic field

- results

- spin-wave velocity

$$\frac{c_-^2}{c_0^2} \approx 1 - \frac{6\sqrt{3} \tilde{h}^2}{\pi^2 S} \ln \left(\frac{2}{\tilde{h}} \right)$$

$$D = 3$$

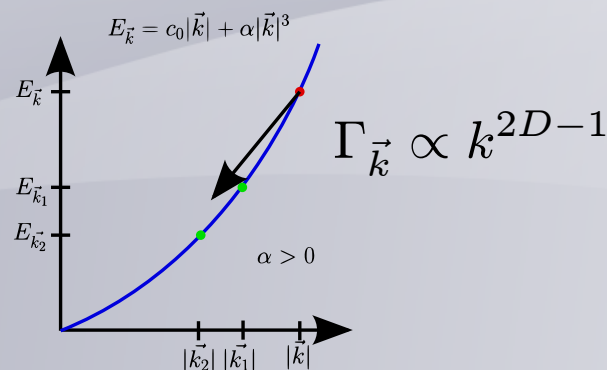
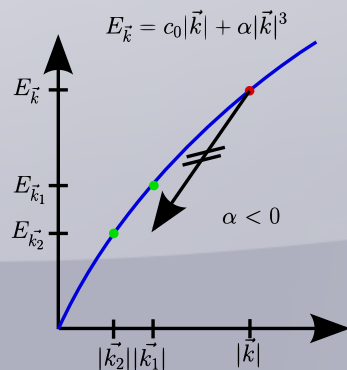
$$\frac{c_-^2}{c_0^2} \approx 1 - \frac{2\tilde{h}}{\pi S} \quad D = 2$$

$$\tilde{h} = \frac{h}{\Delta_0}$$

nonanalytic in $\hbar^2$

- magnon damping

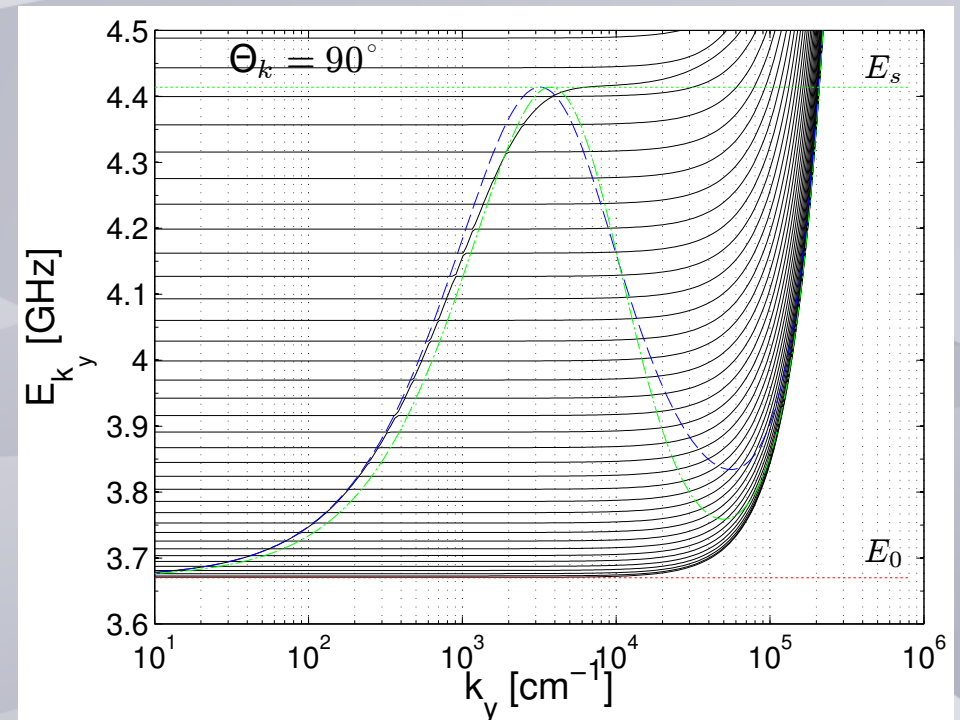
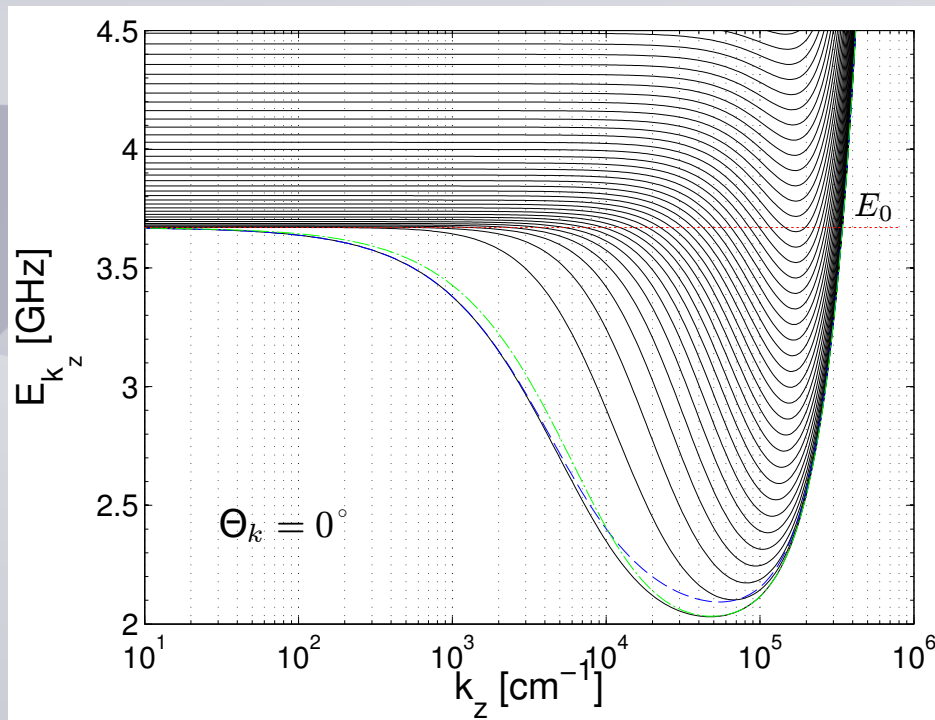
$$\Gamma_{\vec{k}-} \propto \frac{1}{S} \left(\frac{h}{h_c} \right)^2 \left(\sqrt{6\bar{A}_-} \right)^{D-3} a^{D+1} |\vec{k}|^{2D-1}$$



6.5 Theoretical details

Spin-wave theory for thin films

- spectrum for realistic samples



$$d = 4040a \quad H_e = 700 \text{ Oe}$$

6.6: Theoretical details

Spin-wave theory for thin films

- Comparison $E_{\vec{k}} = \sqrt{[h + \rho_{\text{ex}} \vec{k}^2 + \Delta(1 - f_{\vec{k}}) \sin^2 \Theta_{\vec{k}}][h + \rho_{\text{ex}} \vec{k}^2 + \Delta f_{\vec{k}}]}$
 - analytical result

- uniform mode approximation

$$f_{\vec{k}} = \frac{1 - e^{-|\vec{k}|d}}{|\vec{k}|d} \quad \Delta = 4\pi\mu M_S$$

- eigenmode approximation

$$f_{\vec{k}} = 1 - |\vec{k}d| \frac{|\vec{k}d|^3 + |\vec{k}d|\pi^2 + 2\pi^2(1 + e^{-|\vec{k}d|})}{(\vec{k}^2 d^2 + \pi^2)^2}$$

- numerical result

