# Heisenberg Model for Semi-Infinite Systems

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# Outline

- Motivation
- Heisenberg Model and Magnetic Exchange
- Magnons and Spin Waves
- Surfaces in Semi-Infinite Systems
- Examples

# Motivation

- bulk symmetry broken by surface
  - no Fourier transform between layers
  - change in electrical and magnetic properties

| $J_1$ BCC Fe | Bulk | Surface |
|---|---|---|
| $(001)$ | $11.51$ meV | $1.31$ meV |
| $(011)$ | $12.68$ meV | $24.89$ meV |
| $(111)$ | $-1.68$ meV | $1.66$ meV |

- surface (& interface) properties decisive
  - Superconductivity (Pnictides)
  - Magnonics

# Motivation - Magnonics

- information transport & manipulation using magnons
- lower power consumption possible (no motion of electric charges)
- wide range of wavelengths

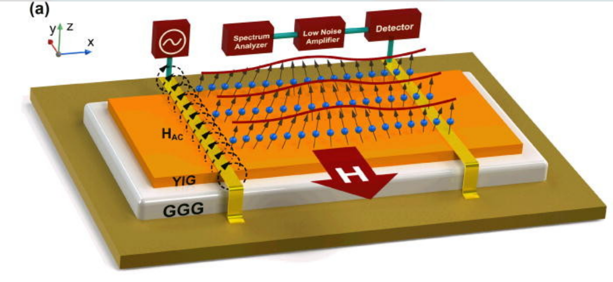


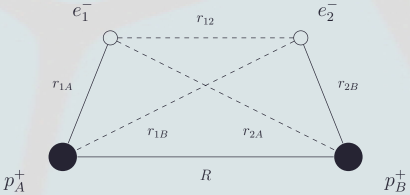

Image Source: S. Rumyantsev et. al. The discrete noise of magnons. `https://doi.org/10.1063/1.5088651`

# Magnetic Exchange - Introductory Model: $H_2$

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{1A} + \hat{\mathcal{H}}_{2B} - \frac{e^2}{4\pi\varepsilon_0 r_{1B}} - \frac{e^2}{4\pi\varepsilon_0 r_{2A}} + \frac{e^2}{4\pi\varepsilon_0 R} + \frac{e^2}{4\pi\varepsilon_0 r_{12}}$$

- for $R \to \infty$:

$$\hat{\mathcal{H}}_{1A}\phi_A^{(1)} = E_0\phi_A^{(1)}$$
$$\hat{\mathcal{H}}_{2B}\phi_B^{(2)} = E_0\phi_B^{(2)}$$



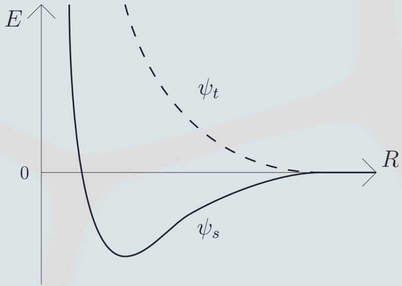

- approximate solution using a variational approach

$$E = \frac{\langle\psi|\hat{\mathcal{H}}|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_{ground}$$

# $H_2$ - Preferred Spin State

$$|\psi_s\rangle = |\psi_+\rangle\,|0\,m\rangle$$
$$|\psi_t\rangle = |\psi_-\rangle\,|1\,m\rangle$$

- analysing energy with varying $R \Rightarrow \psi_s$ preferred
- preferred spin configuration *without* explicit usage of $|S\,m\rangle$




can we describe the problem using *only* spin?

$$\hat{\mathcal{H}}_s = \underbrace{\frac{1}{4}(E_+ + 3E_-)}_{J_0} - \underbrace{\frac{1}{\hbar^2}(E_+ - E_-)}_{J_{12}}\left(\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2\right)$$

# Heisenberg Model

- postulate model for $N$ spins:

$$\hat{\mathcal{H}} = -\sum_{i,j} J_{ij} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$

- *direct* exchange:
  - overlap of wavefunctions leads to magnetic interaction
  - applicable to $e^- \leftrightarrow e^-$ ($H_2$), $e^- \leftrightarrow p^+$,...
  - strength scales as $e^{-x}$ with distance
- *indirect* exchange:
  - no direct overlap between sites
  - coupling through intermediate contributors
  - far reaching interaction
- easily extended with further terms
  - external field, anisotropy terms,...

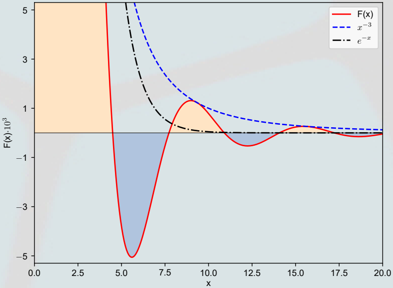
# Indirect Exchange - RKKY

- predominant exchange in many metals (Fe, Nd, Sc,...)

- 'sea' of conduction electrons

$$\hat{\mathcal{H}}_{cond.} = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma}$$

- direct exchange between mobile $e^-$ and localized ions




$$\hat{\mathcal{H}} = -\sum_{i,j} J_{ij}^{RKKY} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \quad , \; J_{ij}^{RKKY} \propto F(2k_F|\mathbf{R}_i - \mathbf{R}_j|)$$

# Heisenberg Model - Ground State

$$\hat{\mathcal{H}} = -\sum_{i,j} J_{ij} \left( \hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^z \hat{S}_j^z \right)$$

- ferromagnetic interaction: $J_{ij} > 0$
  - lower bound for ground state energy:

$$|\phi\rangle = \prod_i |S,\, m_i\rangle_i \quad \Longrightarrow \quad \langle\phi|\hat{\mathcal{H}}|\phi\rangle \geq -\hbar^2 S^2 \sum_{i,j} J_{ij}$$

  - fully aligned state

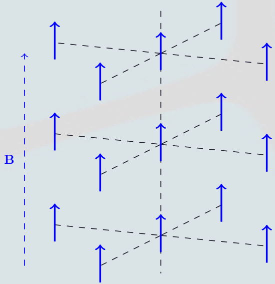
$$|0\rangle = \prod_i |S, \pm S\rangle_i \quad \Longrightarrow \quad \hat{\mathcal{H}}\,|0\rangle = -\hbar^2 S^2 \sum_{i,j} J_{ij}\,|0\rangle$$

# Momentum Space

- external magnetic field sets 'easy' axis $$\hat{\mathcal{H}}_{\mathbf{B}} = -b_0 \sum_i \hat{S}_i^z$$
- Fourier transforms

$$\hat{S}^{(x,y,z,\pm)}(\mathbf{k}) = \sum_i \hat{S}_i^{(x,y,z,\pm)} e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i}$$

$$J(\mathbf{k}) = \frac{1}{N} \sum_{i,j} J_{ij} e^{\mathrm{i}\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}$$




$$\Longrightarrow \hat{\mathcal{H}} = -\frac{1}{N} \sum_{\mathbf{k}} J(\mathbf{k}) \left[\hat{S}^+(\mathbf{k})\hat{S}^-(-\mathbf{k}) + \hat{S}^z(\mathbf{k})\hat{S}^z(-\mathbf{k})\right] - b_0 \hat{S}^z(\mathbf{0})$$

# Quasiparticle View - Magnons

- excited 'one-magnon states'

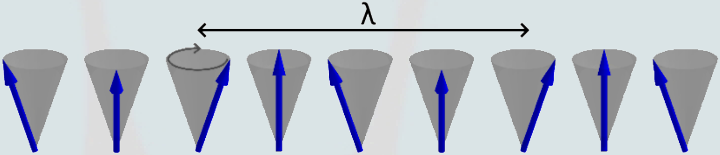
$$|\mathbf{k}\rangle = \frac{1}{\hbar^2\sqrt{2SN}}\hat{S}^-(\mathbf{k})\,|0\rangle \quad , \; E(\mathbf{k}) = E_0 + \hbar\omega(\mathbf{k})$$

- excitation energy

$$\hbar\omega(\mathbf{k}) = b_0\hbar + 2S\hbar^2[J(\mathbf{0}) - J(\mathbf{k})]$$

- the 'spin-flip' is distributed throughout the system

$$\langle\mathbf{k}|\hat{S}_i^z|\mathbf{k}\rangle = \hbar S - \frac{\hbar}{N}$$



# Equation of Motion - Semi Classical

- unit magnetic moments

$$\mathbf{e}_i = \mathbf{m}_i |m_i|^{-1}$$

- effective magnetic field

$$\mathbf{B}_{eff} = \frac{1}{\mu_B |m_i|} \sum_j J_{ij} \mathbf{e}_j$$

- equation of motion for spins

$$|m_i| \partial_t \mathbf{e}_i = -g\mu_B |m_i| \mathbf{e}_i \times \mathbf{B}_{eff}$$

- EOM becomes linear assuming small deviations $e_i^+$

$$|m_i| \partial_t e_i^+(t) = g\mathfrak{i} \sum_j J_{ij} \left( e_i^+ e_j - e_i e_j^+ \right)$$

- translational symmetry *in* layers intact

$$e_{il}^+(t) = e_l^+(\mathbf{k}) e^{\mathfrak{i}\mathbf{k}\cdot\mathbf{R}_i} e^{\mathfrak{i}\omega t}$$

# Torque Matrix

- ansatz results in eigenvalue problem

$$\boxed{\omega_l e_l^+ = \sum_m T_{lm} e_m^+}$$

- torque matrix $\mathbf{T}$

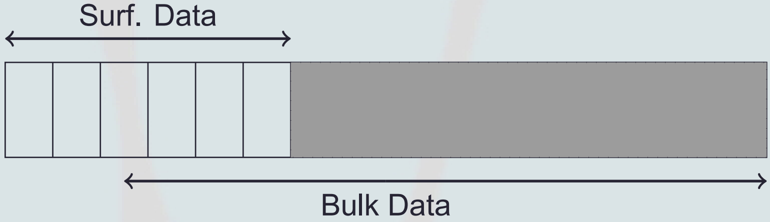
$$T_{lm} = \frac{g}{|m_l|}\left[\delta_{lm}\sum_{m'} J_{l(m')}(\mathbf{0}) - J_{(l)m}(\mathbf{k})\right]$$

$$J_{l(m)}(\mathbf{0}) = \sum_j e_{jm} J_{iljm} \; ; \quad J_{(l)m}(\mathbf{k}) = e_{il}\sum_j J_{iljm} e^{\mathbf{i}\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)}$$

# Semi-Infinite Systems

- banded, *infinite* matrix
- limited number of distinct layers $L_n$ above bulk $B$
- terminate matrix after sufficient number of bulk layers

$$\mathbf{T} = \begin{bmatrix} L_0 & \alpha & & & & \\ \alpha & L_1 & \beta & & & \\ & \beta & B & \gamma & & \\ & & \gamma & B & \gamma & \\ & & & \gamma & B & \\ & & & & & \ddots \end{bmatrix}$$

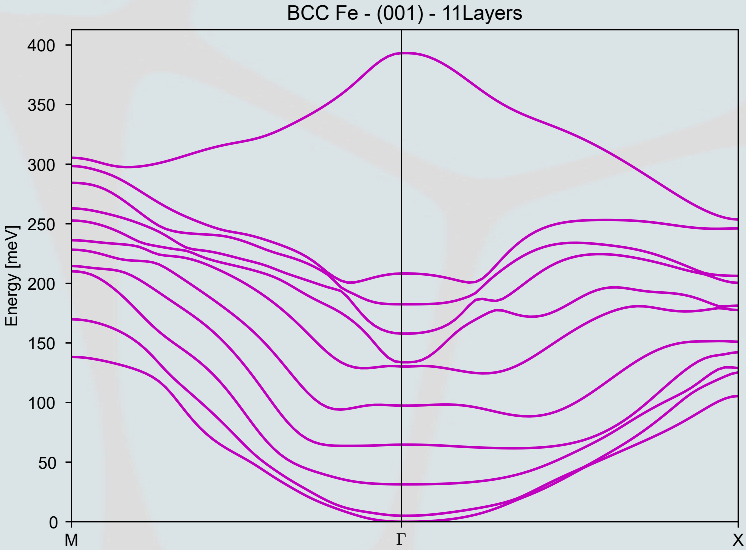


# Exchange Parameters from First Principle

- calculation from scattering quantities by the magnetic force theorem
  - map energy change from perturbation of spins at different lattice sites using Green's functions
  - needed scattering quantities are found during calculations of electronic structure
- calculation from Total Energy Differences
  - mapping of energy differences of spin configurations
  - linear equations for $J_{ij}$ but feasibility limited by range of interaction
- exchange in NiO [meV]

| | Exp. | MFT | ΔE |
|---|---|---|---|
| $J_1$ | $0.69$ | $0.15$ | $1.44$ |
| $J_2$ | $-9.51$ | $-6.92$ | $-6.95$ |

# Examples - BCC Fe (001)

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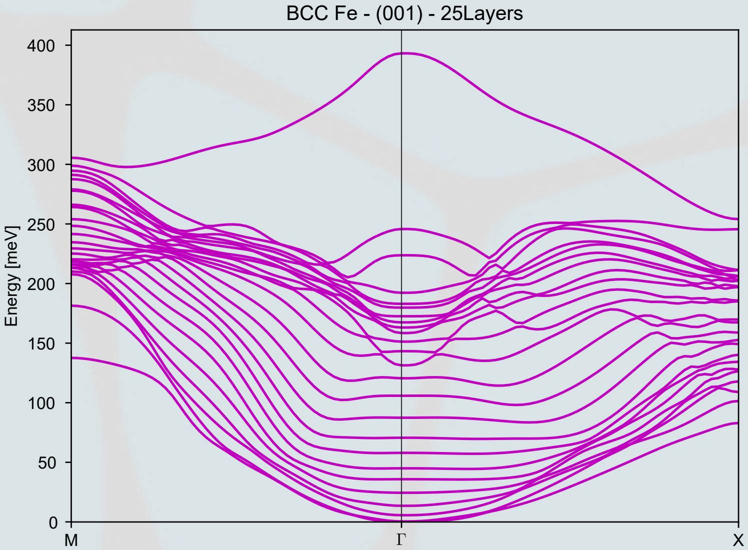

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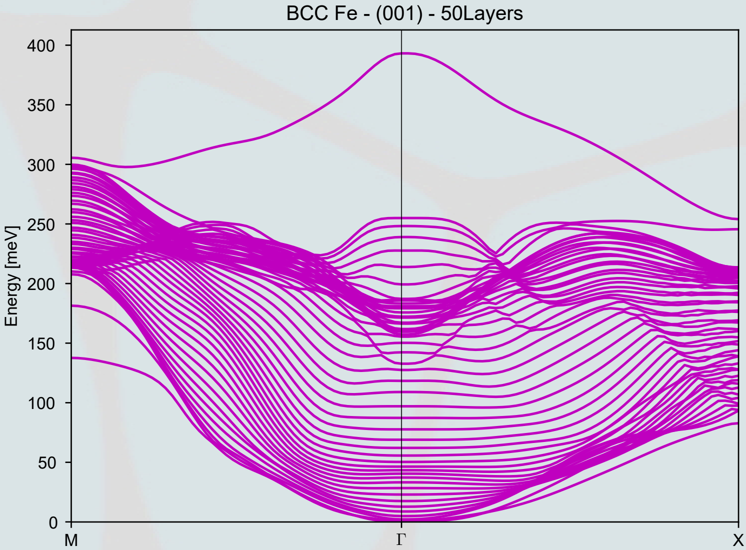

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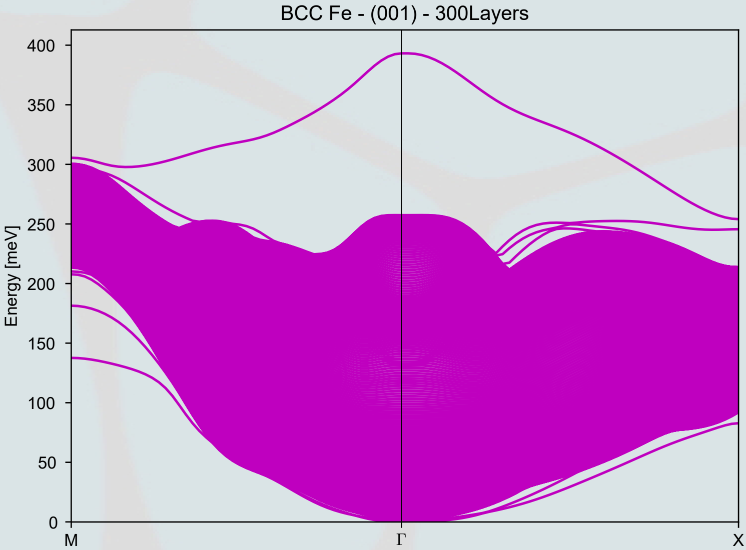
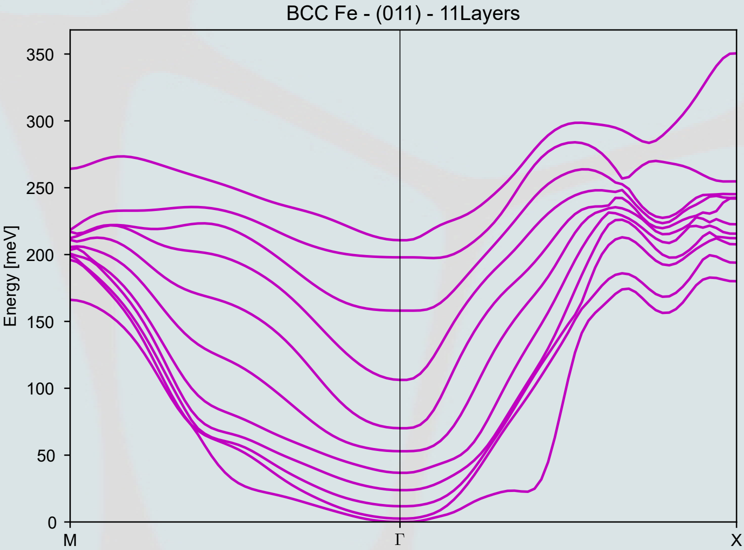
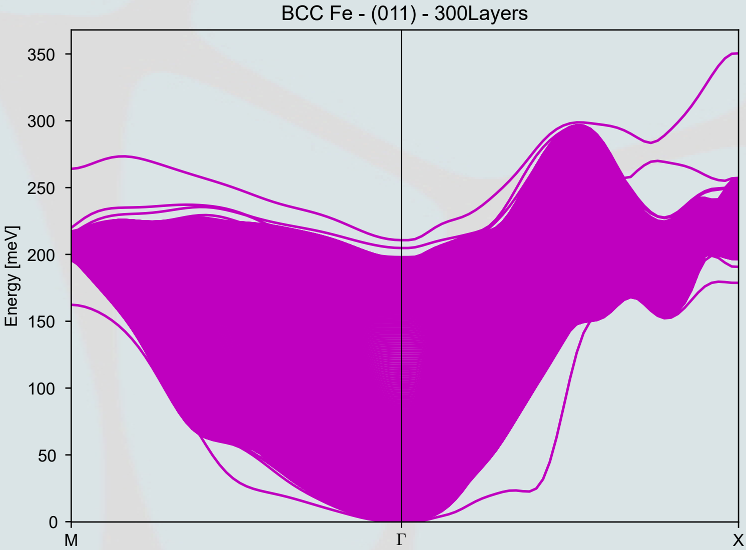


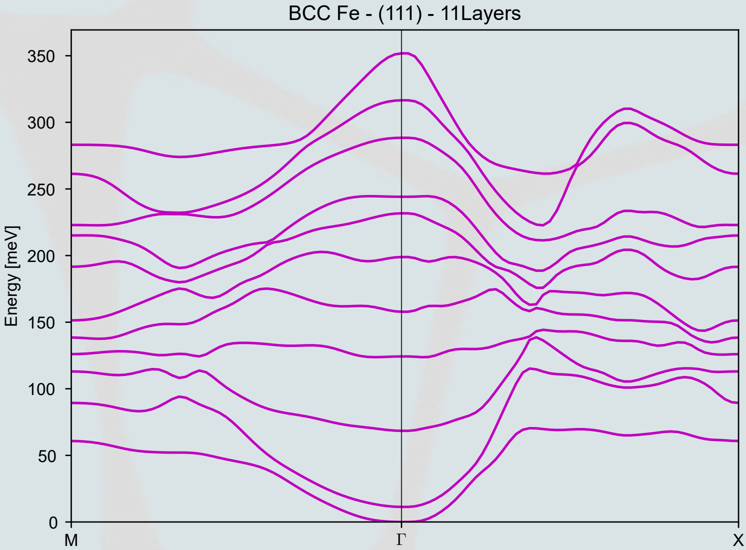
# Examples - BCC Fe (011)



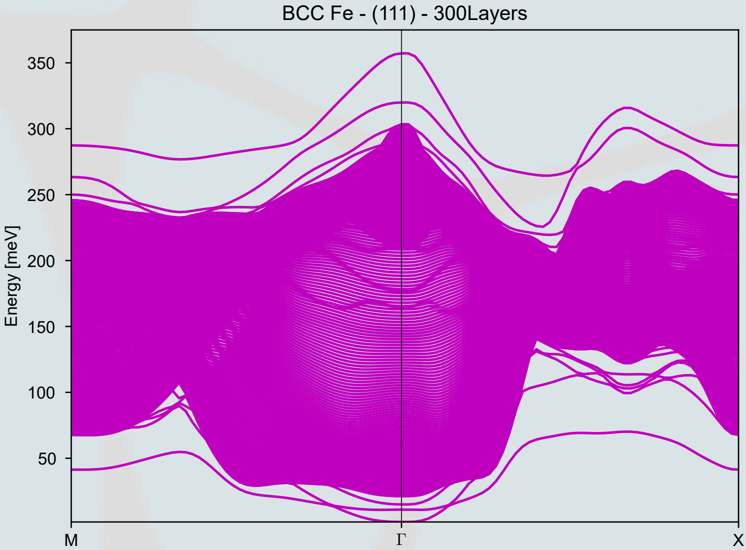
# Examples - BCC Fe (011)



# Examples - BCC Fe (111)



# Examples - BCC Fe (111)



# Summary

- symmetry breaking at surface can strongly change magnetic properties of the system
- surface behaviour is important in applications like Magnonics
- adapted previous methods to obtain spin wave energies resolved in layers
- combined bulk and surface data from ab initio calculations to find dispersion of semi-infinite systems

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