Heisenberg model

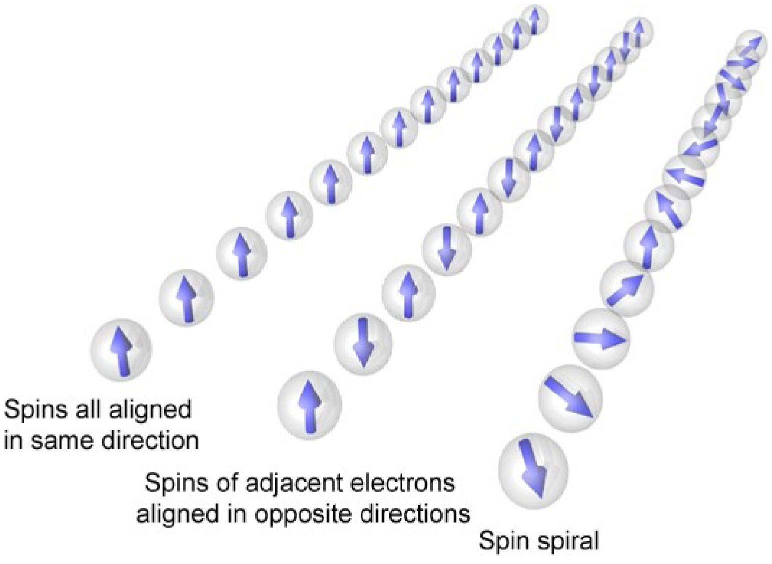
- Generalization of the situation with hydrogen molecule:

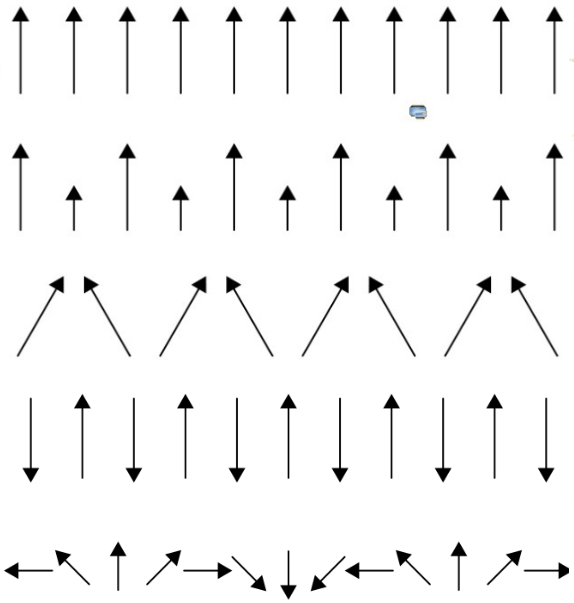
$$\hat{H} = -\sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

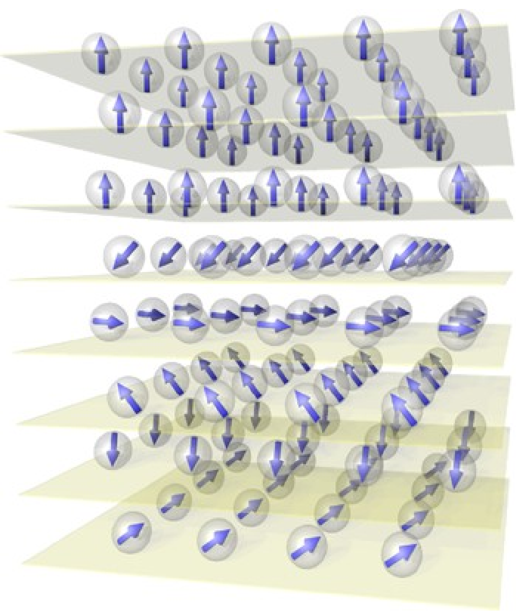
- Extracting J_{ij} is not a trivial problem and to some extent it is still not completely solved
- Solving the quantum model itself without approximations is computationally unsolvable except for smallest systems
- Mechanisms/sources of J_{ij} (Olle's lecture next week):
  - Direct exchange
  - Super-exchange
  - Indirect exchange (RKKY)
  - Itinerant exchange

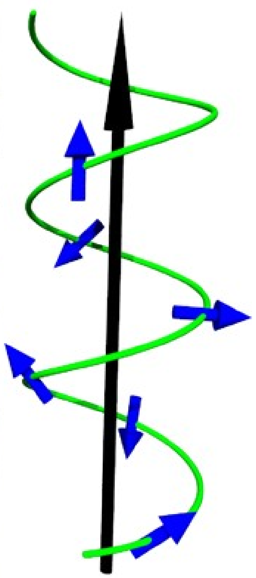
Magnetic structures

- J>0 for nearest neighbors → ferromagnet
- J<0 for nearest neighbors → antiferromagnet
- non-negligible J's for more distant neighbors or in geometries leading to magnetic frustrations → more complicated magnetic structures, e.g., spin spirals, non-collinear structures, etc.









Mean-field theory – Weiss field

- rewrite the Heisenberg model, including field:

$$\hat{H} = -\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j + \sum_i g\mu_B \mathbf{S}_i \cdot \mathbf{H} = -\sum_i \mathbf{S}_i \cdot \left[\sum_j J_{ij}\mathbf{S}_j + g\mu_B \mathbf{H}\right]$$

- this looks like a set of spins in *effective* field

$$\hat{H} = -g\mu_B \sum_i \mathbf{S}_i \cdot \mathbf{H}_i^{\mathrm{eff}} \quad \text{with} \quad \mathbf{H}_i^{\mathrm{eff}} = \mathbf{H} + \frac{1}{g\mu_B}\sum_j J_{ij}\mathbf{S}_j$$

  which does not depend on *i* due to periodicity

- yet, the effective (Weiss) field is an operator → the mean-field theory replaces it with its thermodynamic mean value

$$\mathbf{H}^{\mathrm{eff}} = \mathbf{H} + \lambda\mathbf{M} \quad \text{where} \quad \lambda = \frac{V}{N}\frac{\sum_i J_{i0}}{(g\mu_B)^2} \quad \text{and} \quad \mathbf{M} = \frac{N}{V} g\mu_B \langle \mathbf{S}_0 \rangle$$

Critical temperature

- Taking mean-field approximation and zero external field we obtain equation

$$M(T) = \frac{N}{V} g\mu_B J B_J(\beta g\mu_B J H^{\mathrm{eff}}) = \frac{N}{V} g\mu_B J B_J(\beta g\mu_B J\lambda M(T))$$

- When $M(T)$ goes to zero, $B_J(x) \approx \frac{J+1}{3J} x$ and we get

$$M(T) = \frac{J(J+1)\sum_i J_{i0}}{3k_B T_C} M(T) \quad \rightarrow \quad T_C = \frac{J(J+1)}{3k_B} \sum_i J_{i0}$$

  the mean-field approximation of the magnetic transition temperature

- Weak points: over-estimation of T_C, wrong low-temperature behavior, also around T_C

More advanced methods

- Random-phase approximation

$$\left(k_{\mathrm{B}} T_{\mathrm{C}}^{\mathrm{RPA}}\right)^{-1} = \frac{3}{2} \frac{1}{N} \sum_{\mathbf{q}} \left[J^0 - J(\mathbf{q})\right]^{-1}$$

- Monte-Carlo simulations – exact answers within the classical Heisenberg model, though demanding calculations
- Using numerical methods we can also get *M*(*T*) within all three methods
- Doing Monte-Carlo Heisenberg model quantum-mechanically is still an active field of research

Ground state of ferromagnet

- At T=0, all moments aligned parallel, i.e., total moment NS → |NS,NS>
- Rewrite Heisenberg Hamiltonian using raising and lowering operators:

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y \qquad \hat{S}_\pm|S, S_z\rangle = \sqrt{(S \mp S_z)(S + 1 \pm S_z)}|S, S_z \pm 1\rangle$$

$$\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j = \hat{S}_x^{(i)}\hat{S}_x^{(j)} + \hat{S}_y^{(i)}\hat{S}_y^{(j)} + \hat{S}_z^{(i)}\hat{S}_z^{(j)} = \frac{1}{2}\left(\hat{S}_+^{(i)}\hat{S}_-^{(j)} + \hat{S}_-^{(i)}\hat{S}_+^{(j)}\right) + \hat{S}_z^{(i)}\hat{S}_z^{(j)}$$

- Applying the HH on the |NS,NS> gives

$$\hat{H}|NS, NS\rangle = \left(-\sum_{i\neq j} J_{ij}S^2 - Ng\mu_B SH\right)|NS, NS\rangle \equiv E_0|0\rangle$$

i.e., it is an eigenstate of the HH

- No lower energy-state of ferromagnetic HH exists → it is a ground state |0>

Hint: $\langle\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j\rangle \leq S^2 \quad \text{if} \quad i \neq j$

$$\hat{H} = -\sum_{ij} J_{ij}\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - g\mu_B H \sum_i \hat{s}_z^{(i)}$$

Low-T excitations of ferromagnet

- Lowering spin projection by one at one site is not an eigenstate of HH:

$$\hat{H}|i\rangle = (E_0 + g\mu_B H)\,|i\rangle + 2S\sum_j J_{ij}\,(|i\rangle - |j\rangle)$$

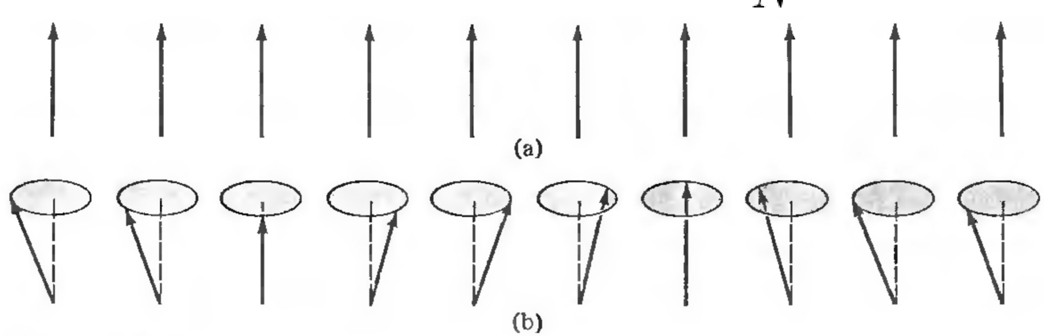
- Because $J_{ij} \equiv J(\mathbf{R}_i, \mathbf{R}_j) = J(\mathbf{R}_i - \mathbf{R}_j)$, i.e., translational invariance, we can construct linear combinations

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{N}}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}|i\rangle$$

which *are eigenstates* of Heisenberg Hamiltonian:

$$\hat{H}|\mathbf{k}\rangle = \left[E_0 + g\mu_B H + 2S\sum_i J_{i0}\left(1 - e^{i\mathbf{k}\cdot\mathbf{R}_i}\right)\right]|\mathbf{k}\rangle \equiv E_{\mathbf{k}}|\mathbf{k}\rangle$$

- One can show that $\langle\mathbf{k}|\hat{S}_x^{(i)}\hat{S}_x^{(j)} + \hat{S}_y^{(i)}\hat{S}_y^{(j)}|\mathbf{k}\rangle = \dfrac{2S}{N}e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)}$



Low temperature magnetization

- Superposition of magnons (like for phonons) is only an approximation here, but “quite OK” for low-lying excited states

$$E = \sum_{\mathbf{k}} E_{\mathbf{k}} n_{\mathbf{k}} \qquad n_{\mathbf{k}} = \frac{1}{e^{E_{\mathbf{k}}/k_B T} - 1}$$

- The magnetization is reduced by one per magnon, i.e.

$$M(T) = M(0)\left[1 - \frac{1}{NS}\sum_{\mathbf{k}} n_{\mathbf{k}}\right] = M(0)\left[1 - \frac{V}{NS}\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{e^{E_{\mathbf{k}}/k_B T} - 1}\right]$$

- At low temperatures only the lowest energy excitations happen, and for these $E_{\mathbf{k}} = E_0 + g\mu_B H + \frac{S}{2}\sum_i J_{i0}(\mathbf{k}\cdot\mathbf{R}_i)^2$ i.e.,

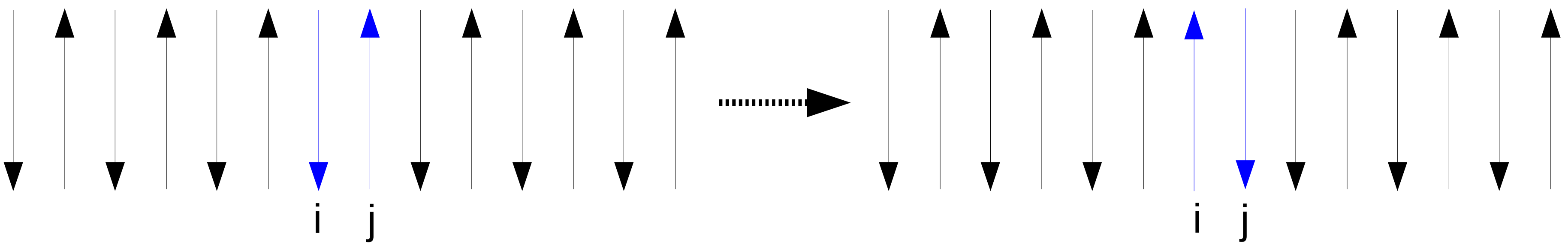
$$M(T) = M(0)\left[1 - \frac{V}{NS}(k_B T)^{\frac{3}{2}}\int \frac{d\mathbf{q}}{(2\pi)^3}\left(\exp\frac{S\sum_i J_{i0}(\mathbf{q}\cdot\mathbf{R}_i)^2}{2} - 1\right)^{-1}\right]$$

  Bloch's 3/2 law

- Mermin-Wagner theorem → no magnetization in 2D or 1D

Ground state of antiferromagnet

- Intuitively: arrangement of alternating up/down moments
- It is *not* an eigenstate of Heisenberg Hamiltonian!
- Assume S=1/2 chain and apply $\hat{S}_{+}^{(i)}\hat{S}_{-}^{(j)}$



- In classical case (spins as vectors) this is a ground state with lowest energy
- For nearest-neighbor (NN) interaction the following bounds are valid:

$$-S(S+1)\sum_{NN}|J_{ij}| \leq E_0 \leq -S^2\sum_{NN}|J_{ij}|$$

which actually coincide in the classical case, where $S \to \infty$