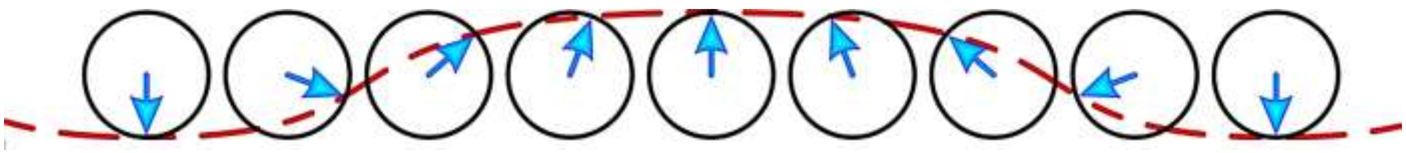
Fenómenos Colectivos en Sólidos

Ondas de Espín (Magnones)



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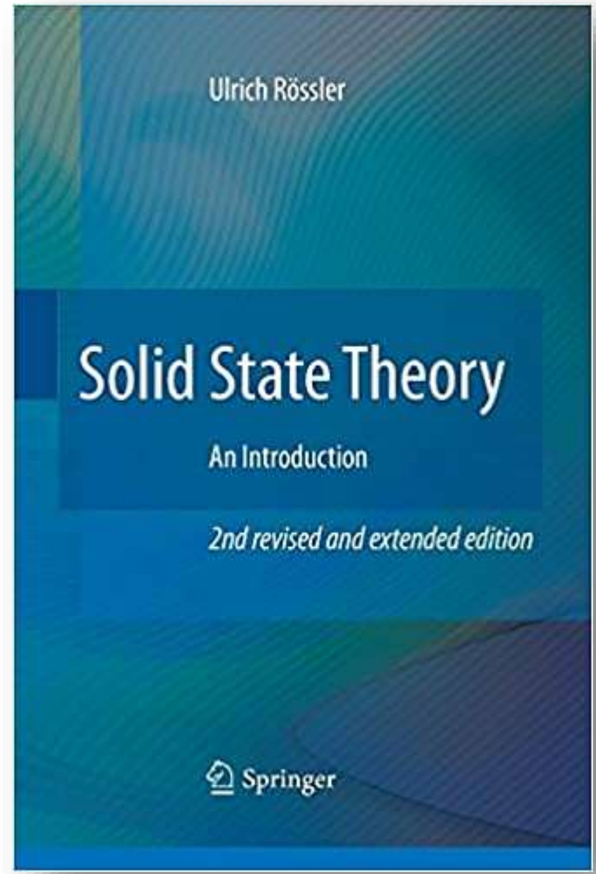
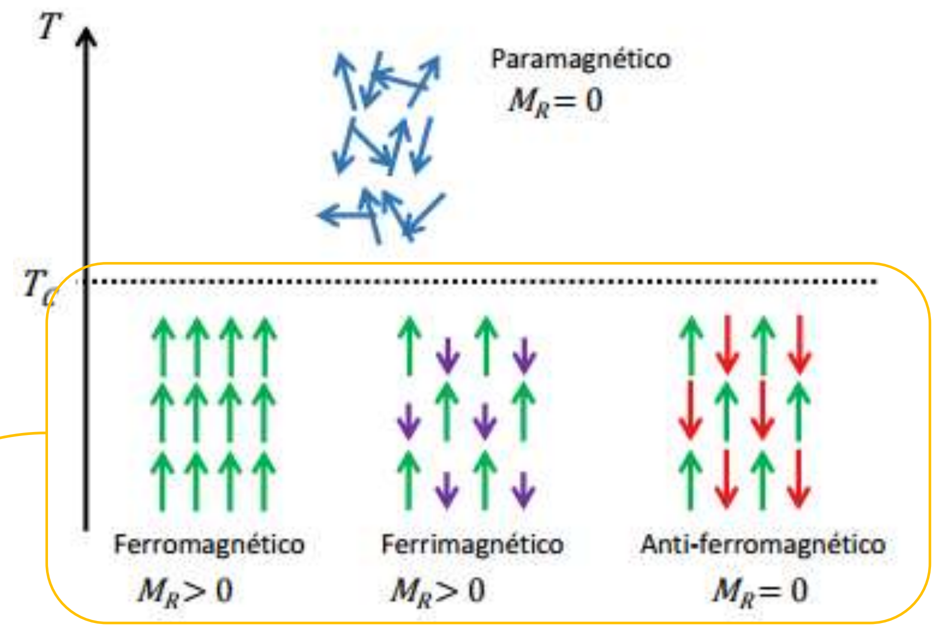
Julio de 2021

Bibliografía



Modelo de Heisenberg

Magnetismo ⇨ Materiales con orbitales *d* o *f* incompletos



Magnetización espontánea → **Mecanismos de intercambio** que favorecen la alineación de los momentos magnéticos

- **Interacción Coulombiana**
- **Principio de exclusión de Pauli**

Modelo de Heisenberg

Magnetismo ⇨ Materiales con orbitales *d* o *f* incompletos

Los electrones forman bandas estrechas → **Aproximación tight-binding**

Partimos del Hamiltoniano de *N* electrones en un potencial periódico:

$$\mathcal{H} = \sum_{\alpha} \epsilon_\alpha c_\alpha^\dagger c_\alpha + \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} V_{\alpha\beta\beta'\alpha'} c_\alpha^\dagger c_\beta^\dagger c_{\alpha'} c_{\beta'}$$

donde $\alpha = n\boldsymbol{k}\sigma$

Nº cuánticos de estados de Bloch

$$V_{\alpha\beta\beta'\alpha'} = \int \mathrm{d}x \int \mathrm{d}x' \psi_\alpha^\dagger(x) \psi_\beta^\dagger(x') \frac{e^2}{4\pi\varepsilon_0 |\boldsymbol{r} - \boldsymbol{r}'|} \psi_{\beta'}(x) \psi_{\alpha'}(x')$$

Consideramos la función de Bloch de los electrones en una banda derivada de tales orbitales:

$$\psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \phi_\sigma(\boldsymbol{r} - \boldsymbol{R}) \longrightarrow c_{\boldsymbol{k}\sigma} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} c_{\boldsymbol{R}\sigma}$$

Representación de Wannier

Modelo de Heisenberg

Partimos del Hamiltoniano de *N* electrones en un potencial periódico:

$$\mathcal{H} = \sum_{\alpha} \epsilon_{\alpha} c_{\alpha}^{\dagger} c_{\alpha} + \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} V_{\alpha\beta\beta'\alpha'} c_{\alpha}^{\dagger} c_{\beta}^{\dagger} c_{\alpha'} c_{\beta'}$$

$$= \mathcal{H}_{\text{sp}} + \mathcal{H}_{\text{int}}$$

Interaction

Single-particle

$$\mathcal{H}_{\text{sp}} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^{\dagger} c_{\boldsymbol{k}\sigma}$$

$$= \sum_{\boldsymbol{R}\boldsymbol{R}'\sigma} \underbrace{\frac{1}{N} \sum_{\boldsymbol{k}} \epsilon_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}_{t_{\boldsymbol{R}\boldsymbol{R}'}} c_{\boldsymbol{R}'\sigma}^{\dagger} c_{\boldsymbol{R}\sigma} = \sum_{\boldsymbol{R}\boldsymbol{R}'\sigma} t_{\boldsymbol{R}\boldsymbol{R}'} c_{\boldsymbol{R}'\sigma}^{\dagger} c_{\boldsymbol{R}\sigma}$$

$t_{\boldsymbol{R}\boldsymbol{R}'}$ → Dispersión de la energía $\epsilon_{\boldsymbol{k}}$ de la banda

En el caso de **orbitales fuertemente localizados** $\longrightarrow$ $t_{\boldsymbol{R}\boldsymbol{R}'} = 0$ para $\boldsymbol{R} \neq \boldsymbol{R}'$

Modelo de Heisenberg

Partimos del Hamiltoniano de *N* electrones en un potencial periódico:

$$\mathcal{H} = \sum_{\alpha} \epsilon_\alpha c_\alpha^\dagger c_\alpha + \frac{1}{2} \sum_{\alpha\beta\alpha'\beta'} V_{\alpha\beta\beta'\alpha'} c_\alpha^\dagger c_\beta^\dagger c_{\alpha'} c_{\beta'}$$

$$= \mathcal{H}_{\text{sp}} + \mathcal{H}_{\text{int}}$$

Interaction

Single-particle

$$\mathcal{H}_{\text{int}} = \frac{1}{2} \sum_{\substack{\boldsymbol{R}_1 \boldsymbol{R}_2 \sigma \\ \boldsymbol{R}_1' \boldsymbol{R}_2' \sigma'}} V_{\boldsymbol{R}_1 \boldsymbol{R}_2 \boldsymbol{R}_1' \boldsymbol{R}_2'} c_{\boldsymbol{R}_1 \sigma}^\dagger c_{\boldsymbol{R}_2 \sigma'}^\dagger c_{\boldsymbol{R}_2' \sigma'} c_{\boldsymbol{R}_1' \sigma}$$

$$V_{\boldsymbol{R}_1 \boldsymbol{R}_2 \boldsymbol{R}_1' \boldsymbol{R}_2'} = \int \mathrm{d}^3 \boldsymbol{r} \int \mathrm{d}^3 \boldsymbol{r}' \phi^*(\boldsymbol{r} - \boldsymbol{R}_1) \phi^*(\boldsymbol{r}' - \boldsymbol{R}_2) \times \frac{e^2}{4\pi\varepsilon_0 |\boldsymbol{r} - \boldsymbol{r}'|} \phi(\boldsymbol{r} - \boldsymbol{R}_1') \phi(\boldsymbol{r}' - \boldsymbol{R}_2').$$

Note, that the Wannier (or atomic) orbitals and the single particle energies are assumed to be independent of the spin quantum number σ. This means to neglect all spin-dependent effects deriving from spin–orbit coupling and from the electrons in all other occupied bands of the solid, while here all spin related effects derive from the interaction term.

Modelo de Heisenberg

$$\mathcal{H}_{\text{int}} = \frac{1}{2} \sum_{\substack{\boldsymbol{R}_1 \boldsymbol{R}_2 \sigma \\ \boldsymbol{R}_1' \boldsymbol{R}_2' \sigma'}} V_{\boldsymbol{R}_1 \boldsymbol{R}_2 \boldsymbol{R}_1' \boldsymbol{R}_2'} c^\dagger_{\boldsymbol{R}_1 \sigma} c^\dagger_{\boldsymbol{R}_2 \sigma'} c_{\boldsymbol{R}_2' \sigma'} c_{\boldsymbol{R}_1' \sigma}$$

Aproximación de HF

2 términos

Directo — **Intercambio**

Término Directo ⇒ $\boldsymbol{R}_1 = \boldsymbol{R}_1' = \boldsymbol{R}$ and $\boldsymbol{R}_2 = \boldsymbol{R}_2' = \boldsymbol{R}'$

$$\mathcal{H}_{\text{d}} = \frac{1}{2} \sum_{\boldsymbol{R}\boldsymbol{R}'} V_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}\boldsymbol{R}'} \sum_{\sigma\sigma'} c^\dagger_{\boldsymbol{R}\sigma} c^\dagger_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma}$$

$$\left(\sum_{\sigma} c^\dagger_{\boldsymbol{R}\sigma} c_{\boldsymbol{R}\sigma} \sum_{\sigma'} c^\dagger_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}'\sigma'} = 1 \right)$$

Energía de interacción electrostática entre las densidades de carga localizadas alrededor de ***R*** y ***R´***

Modelo de Heisenberg

$$\mathcal{H}_{\text{int}} = \frac{1}{2} \sum_{\substack{\boldsymbol{R}_1 \boldsymbol{R}_2 \sigma \\ \boldsymbol{R}'_1 \boldsymbol{R}'_2 \sigma'}} V_{\boldsymbol{R}_1 \boldsymbol{R}_2 \boldsymbol{R}'_1 \boldsymbol{R}'_2} c^{\dagger}_{\boldsymbol{R}_1 \sigma} c^{\dagger}_{\boldsymbol{R}_2 \sigma'} c_{\boldsymbol{R}'_2 \sigma'} c_{\boldsymbol{R}'_1 \sigma}$$

Aproximación de HF

2 términos

Directo **Intercambio**

Término de Intercambio $\Rightarrow$ $\boldsymbol{R}_1 = \boldsymbol{R}'_2 = \boldsymbol{R}$ and $\boldsymbol{R}_2 = \boldsymbol{R}'_1 = \boldsymbol{R}'$

$$\mathcal{H}_{\text{x}} = \frac{1}{2} \sum_{\boldsymbol{R}\boldsymbol{R}'} V_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}'\boldsymbol{R}} \sum_{\sigma\sigma'} c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma}$$

$$\sum c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma} = - c^{\dagger}_{\boldsymbol{R}\uparrow} c_{\boldsymbol{R}\uparrow} c^{\dagger}_{\boldsymbol{R}'\uparrow} c_{\boldsymbol{R}'\uparrow} - c^{\dagger}_{\boldsymbol{R}\downarrow} c_{\boldsymbol{R}\downarrow} c^{\dagger}_{\boldsymbol{R}'\downarrow} c_{\boldsymbol{R}'\downarrow} - c^{\dagger}_{\boldsymbol{R}\uparrow} c_{\boldsymbol{R}\downarrow} c^{\dagger}_{\boldsymbol{R}'\downarrow} c_{\boldsymbol{R}'\uparrow} - c^{\dagger}_{\boldsymbol{R}\downarrow} c_{\boldsymbol{R}\uparrow} c^{\dagger}_{\boldsymbol{R}'\uparrow} c_{\boldsymbol{R}'\downarrow}$$

Modelo de Heisenberg

Término de Intercambio

$$\mathcal{H}_{\mathrm{x}} = \frac{1}{2}\sum_{\boldsymbol{R}\boldsymbol{R}'} V_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}'\boldsymbol{R}} \sum_{\sigma\sigma'} c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma}$$

$$\sum c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma} = -\, c^{\dagger}_{\boldsymbol{R}\uparrow} c_{\boldsymbol{R}\uparrow} c^{\dagger}_{\boldsymbol{R}'\uparrow} c_{\boldsymbol{R}'\uparrow} - c^{\dagger}_{\boldsymbol{R}\downarrow} c_{\boldsymbol{R}\downarrow} c^{\dagger}_{\boldsymbol{R}'\downarrow} c_{\boldsymbol{R}'\downarrow} - c^{\dagger}_{\boldsymbol{R}\uparrow} c_{\boldsymbol{R}\downarrow} c^{\dagger}_{\boldsymbol{R}'\downarrow} c_{\boldsymbol{R}'\uparrow} - c^{\dagger}_{\boldsymbol{R}\downarrow} c_{\boldsymbol{R}\uparrow} c^{\dagger}_{\boldsymbol{R}'\uparrow} c_{\boldsymbol{R}'\downarrow}$$

¿Qué significan los productos de estos operadores respecto al sitio **R**?

$c^{\dagger}_{\uparrow}c_{\uparrow},\ c^{\dagger}_{\downarrow}c_{\downarrow}$: count the $\uparrow,\downarrow$ electrons

$c^{\dagger}_{\uparrow}c_{\uparrow} - c^{\dagger}_{\downarrow}c_{\downarrow}$: counts the difference between $\uparrow$ and $\downarrow$ electrons

$c^{\dagger}_{\uparrow}c_{\downarrow},\ c^{\dagger}_{\downarrow}c_{\uparrow}$: cause spin flips.

$[c^{\dagger}_{\uparrow}c_{\downarrow}, c^{\dagger}_{\downarrow}c_{\uparrow}] = c^{\dagger}_{\uparrow}c_{\uparrow} - c^{\dagger}_{\downarrow}c_{\downarrow}$ (Conmutador)

Cumplen con las reglas de conmutación momento angular !!

$$[S^i, S^j] = \mathrm{i}\varepsilon_{ijk}S^k, \quad i,j,k = x,y,z$$

$$S^+ = S^x + \mathrm{i}S^y = c^{\dagger}_{\uparrow}c_{\downarrow},\ S^- = S^x - \mathrm{i}S^y = c^{\dagger}_{\downarrow}c_{\uparrow},\ S^z = \frac{1}{2}(c^{\dagger}_{\uparrow}c_{\uparrow} - c^{\dagger}_{\downarrow}c_{\downarrow})$$

Modelo de Heisenberg

Término de Intercambio

$$\mathcal{H}_{\mathrm{x}} = \frac{1}{2}\sum_{\boldsymbol{R}\boldsymbol{R}'} V_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}'\boldsymbol{R}} \sum_{\sigma\sigma'} c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma}$$

$$\sum c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma} = -\, c^{\dagger}_{\boldsymbol{R}\uparrow} c_{\boldsymbol{R}\uparrow} c^{\dagger}_{\boldsymbol{R}'\uparrow} c_{\boldsymbol{R}'\uparrow} - c^{\dagger}_{\boldsymbol{R}\downarrow} c_{\boldsymbol{R}\downarrow} c^{\dagger}_{\boldsymbol{R}'\downarrow} c_{\boldsymbol{R}'\downarrow} - c^{\dagger}_{\boldsymbol{R}\uparrow} c_{\boldsymbol{R}\downarrow} c^{\dagger}_{\boldsymbol{R}'\downarrow} c_{\boldsymbol{R}'\uparrow} - c^{\dagger}_{\boldsymbol{R}\downarrow} c_{\boldsymbol{R}\uparrow} c^{\dagger}_{\boldsymbol{R}'\uparrow} c_{\boldsymbol{R}'\downarrow}$$

Reescribimos en términos de $\boldsymbol{S}_{\boldsymbol{R}} = (S^{x}_{\boldsymbol{R}}, S^{y}_{\boldsymbol{R}}, S^{z}_{\boldsymbol{R}})$

$$\Rightarrow \sum_{\sigma\sigma'} c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma} = -\left(S^{+}_{\boldsymbol{R}} S^{-}_{\boldsymbol{R}'} + S^{-}_{\boldsymbol{R}} S^{+}_{\boldsymbol{R}'}\right) - 2 S^{z}_{\boldsymbol{R}} S^{z}_{\boldsymbol{R}'} \rightarrow = -\, 2\boldsymbol{S}_{\boldsymbol{R}} \cdot \boldsymbol{S}_{\boldsymbol{R}'}$$

$$-\frac{1}{2}\sum_{\sigma\sigma'} c^{\dagger}_{\boldsymbol{R}\sigma} c_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}'\sigma'} .$$

Se combina con

$$\mathcal{H}_{\mathrm{d}} = \frac{1}{2}\sum_{\boldsymbol{R}\boldsymbol{R}'} V_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}\boldsymbol{R}'} \sum_{\sigma\sigma'} c^{\dagger}_{\boldsymbol{R}\sigma} c^{\dagger}_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma}$$

Modelo de Heisenberg

Hamiltoniano de interacción

$$\mathcal{H}_\mathrm{d} = \frac{1}{2}\sum_{\boldsymbol{R}\boldsymbol{R}'} V_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}\boldsymbol{R}'} \sum_{\sigma\sigma'} c^\dagger_{\boldsymbol{R}\sigma} c^\dagger_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma} \quad + \quad \mathcal{H}_\mathrm{x} = \frac{1}{2}\sum_{\boldsymbol{R}\boldsymbol{R}'} V_{\boldsymbol{R}\boldsymbol{R}'\boldsymbol{R}'\boldsymbol{R}} \sum_{\sigma\sigma'} c^\dagger_{\boldsymbol{R}\sigma} c^\dagger_{\boldsymbol{R}'\sigma'} c_{\boldsymbol{R}\sigma'} c_{\boldsymbol{R}'\sigma}$$

$$\Rightarrow \quad \mathcal{H}_\mathrm{int} = -\sum_{\substack{\boldsymbol{R}\boldsymbol{R}' \\ \boldsymbol{R}\neq\boldsymbol{R}'}} J_{\boldsymbol{R}\boldsymbol{R}'} \boldsymbol{S}_{\boldsymbol{R}} \cdot \boldsymbol{S}_{\boldsymbol{R}'}$$

donde $$J_{\boldsymbol{R}\boldsymbol{R}'} = \int \mathrm{d}^3\boldsymbol{r} \int \mathrm{d}^3\boldsymbol{r}' \frac{e^2 \phi^*(\boldsymbol{r}-\boldsymbol{R})\phi(\boldsymbol{r}-\boldsymbol{R}')\phi^*(\boldsymbol{r}'-\boldsymbol{R}')\phi(\boldsymbol{r}'-\boldsymbol{R})}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}$$ **Integral de intercambio**

Luego, añadimos la contribución de Zeeman y reemplazamos ***R*** por un subíndice *i*

$$\mathcal{H}_\mathrm{spin} = -\sum_{\substack{i,j \\ i\neq j}} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - g\mu_\mathrm{B} H_\mathrm{ext} \sum_i S_i^z$$

Hamiltoniano de Heisenberg

Modelo de Heisenberg

$$\mathcal{H}_{\text{spin}} = -\sum_{\substack{i,j \\ i\neq j}} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - g\mu_{\text{B}} H_{\text{ext}} \sum_i S_i^z$$

Hamiltoniano de Heisenberg

Observaciones:

1) **Distintos modelos:**

1. the anisotropic Heisenberg model

$$\mathcal{H}_{\text{spin}} = -\sum_{\substack{i,j \\ i\neq j}} \left(J_{ij}(S_i^x S_j^x + S_i^y S_j^y) + \bar{J}_{ij} S_i^z S_j^z \right), J_{ij} \neq \bar{J}_{ij},$$

2. the Ising model (with $J_{ij} = 0$)

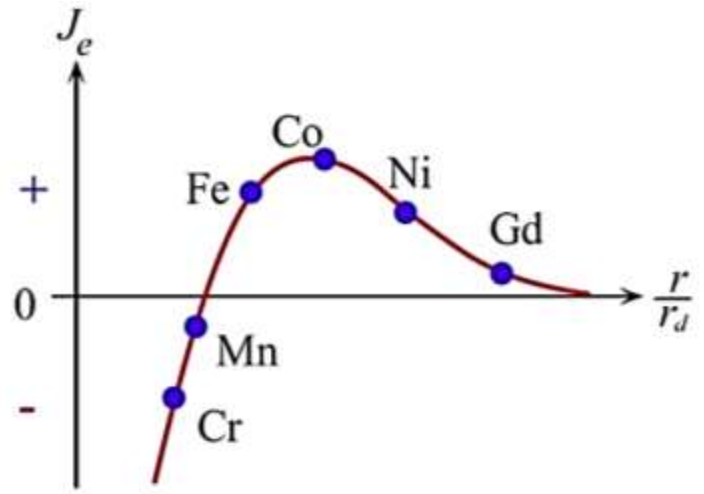
$$\mathcal{H}_{\text{Ising}} = -\sum_{\substack{i,j \\ i\neq j}} \bar{J}_{ij} S_i^z S_j^z,$$

3. and the XY model ($\bar{J}_{ij} = 0$)

$$\mathcal{H}_{XY} = -\sum_{\substack{i,j \\ i\neq j}} J_{ij}(S_i^x S_j^x + S_i^y S_j^y).$$

2) $J_{ij} > 0$ → Conf. **Ferromagnética**

$J_{ij} < 0$ → Conf. **Antiferromagnética**



Ondas de espín

6.3 Spin Waves in Ferromagnets

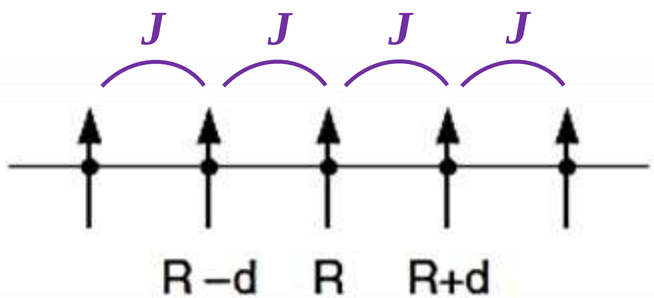
Hamiltoniano de Heisenberg en aproximación tight-binding:

$$\mathcal{H}_{\text{spin}} = -J \sum_{n.n.i,j} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - g\mu_{\text{B}} H_{\text{ext}} \sum_i S_i^z$$

$$= -J \sum_{n.n.i,j} \left\{ \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + S_i^z S_j^z \right\} - g\mu_{\text{B}} H_{\text{ext}} \sum_i S_i^z$$

Interacciones sólo entre primeros vecinos

Una sola integral de intercambio



Ondas de espín

6.3 Spin Waves in Ferromagnets

$$\mathcal{H}_{\text{spin}} = -J \sum_{n.n.i,j} \left\{ \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \right\} - g\mu_B H_{\text{ext}} \sum_i S_i^z.$$

Calculamos la energía del estado fundamental con $H_{ext} = 0$

$$|\Psi_0\rangle = \prod_i |SS\rangle_i$$

$$E_0 = \langle \Psi_0 | \mathcal{H}_{\text{spin}} | \Psi_0 \rangle$$
$$= -J \sum_{n.n.i,j} \langle SS|S_i^z|SS\rangle_i \langle SS|S_j^z|SS\rangle_j = -J\nu S^2 N$$

donde ν = n° de primeros vecinos
N = n° de sitios de la cadena

$$\sum_j S_j^z |\Psi_0\rangle = \sum_j S_j^z \prod_i |SS\rangle_i = NS|\Psi_0\rangle$$

Ondas de espín

6.3 Spin Waves in Ferromagnets

Consideramos de nuevo el hamiltoniano de Heisenberg general:

$$\mathcal{H}_{\text{spin}} = -\sum_{\substack{i,j \\ i\neq j}} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - g\mu_{\text{B}} H_{\text{ext}} \sum_i S_i^z$$

Y analizamos la Ecuación de movimiento de $\boldsymbol{S}_j$:

$$\frac{\mathrm{d}\boldsymbol{S}_j}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\mathcal{H}_{\text{spin}}, \boldsymbol{S}_j] = -\frac{1}{\hbar}(\boldsymbol{H}_j \times \boldsymbol{S}_j)$$

con $\boldsymbol{H}_j = \sum_i J_{ij} \boldsymbol{S}_i + g\mu_{\text{B}} \boldsymbol{H}_{\text{ext}}$

Campo magnético efectivo que actúa sobre el espín $\boldsymbol{S}_j$

Elegimos $\boldsymbol{H}_{ext} = (0,0,H_{ext})$

Ondas de espín

6.3 Spin Waves in Ferromagnets

$$\frac{\mathrm{d}\boldsymbol{S}_j}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\mathcal{H}_{\mathrm{spin}}, \boldsymbol{S}_j] = -\frac{1}{\hbar}(\boldsymbol{H}_j \times \boldsymbol{S}_j) \longrightarrow \hbar\frac{dS_j^z}{dt} = 0$$

$$\hbar\frac{\mathrm{d}S_j^x}{\mathrm{d}t} = -\sum_{n.n.i} J_{ij}\left(S_i^y S_j^z - S_i^z S_j^y\right) + g\mu_{\mathrm{B}} H_{\mathrm{ext}} S_j^y$$

$$\hbar\frac{\mathrm{d}S_j^y}{\mathrm{d}t} = -\sum_{n.n.i} J_{ij}\left(S_i^z S_j^x - S_i^x S_j^z\right) - g\mu_{\mathrm{B}} H_{\mathrm{ext}} S_j^x$$

A **bajas temperaturas** **podemos reemplazar** $S_j^z \rightarrow \langle S_j^z \rangle \simeq S$ (while $\langle S_j^x \rangle, \langle S_j^y \rangle \ll S$)

(cerca del ground state ferromagnético)

$$\Rightarrow \quad \hbar\frac{\mathrm{d}S_j^x}{\mathrm{d}t} = -S\sum_{n.n.i} J_{ij}\left(S_i^y - S_j^y\right) + g\mu_{\mathrm{B}} H_{\mathrm{ext}} S_j^y$$

$$\hbar\frac{\mathrm{d}S_j^y}{\mathrm{d}t} = -S\sum_{n.n.i} J_{ij}\left(S_j^x - S_i^x\right) - g\mu_{\mathrm{B}} H_{\mathrm{ext}} S_j^x$$

$$\hbar\frac{\mathrm{d}S_j^{\pm}}{\mathrm{d}t} = \mp\mathrm{i}\left(S\sum_{n.n.i} J_{ij}(S_j^{\pm} - S_i^{\pm}) + g\mu_{\mathrm{B}} H_{\mathrm{ext}} S_j^{\pm}\right)$$

Ondas de espín

6.3 Spin Waves in Ferromagnets

$$\hbar \frac{\mathrm{d}S_j^{\pm}}{\mathrm{d}t} = \mp \mathrm{i} \left(S \sum_{n.n.i} J_{ij}(S_j^{\pm} - S_i^{\pm}) + g\mu_\mathrm{B} H_\mathrm{ext} S_j^{\pm} \right) \longrightarrow S_{\boldsymbol{k}}^{\pm} = \frac{1}{\sqrt{N}} \sum_j \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} S_j^{\pm}$$

Representación de Bloch

$$\Rightarrow \quad \frac{\hbar}{\mathrm{i}} \frac{\mathrm{d}S_{\boldsymbol{k}}^{\pm}}{\mathrm{d}t} = \left(S \sum_{n.n.i,j} J_{ij} \left(1 - \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\underbrace{(\boldsymbol{R}_i - \boldsymbol{R}_j)}_{\boldsymbol{d}}}\right) + g\mu_\mathrm{B} H_\mathrm{ext} \right) S_j^{\pm}$$

Red cúbica →

($J_{ij} = J$ para los ν pares de n.n.)

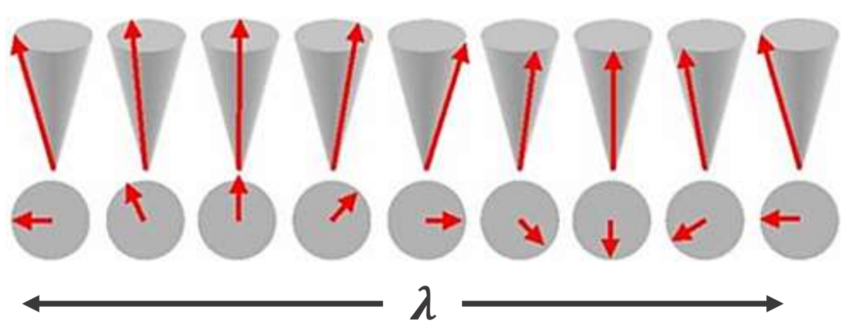
$$\hbar\omega_{\boldsymbol{k}} = 2J\nu S(1 - \gamma_{\boldsymbol{k}}) + g\mu_\mathrm{B} H_\mathrm{ext}, \text{ with } \quad \gamma_{\boldsymbol{k}} = \frac{1}{\nu} \sum_{\boldsymbol{d}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}}$$

Onda de espín

(Magnon)

Frecuencia → $\omega_{\boldsymbol{k}}$

Vector de onda → $\boldsymbol{k}$



Ondas de espín

6.3 Spin Waves in Ferromagnets

Transformación de Holstein-Primakoff → Representación en número de ocupación

¿Cuánto se desvía S_j^z de su valor máximo S?

Se reemplazan los operadores $S_j^{\pm}$ por operadores bosónicos $a_j^{\dagger}, a_j$ mediante:

$$S_j^+ = \sqrt{2S}\left\{1 - \frac{1}{2S}a_j^{\dagger}a_j\right\}^{1/2} a_j, \quad S_j^- = \sqrt{2S}a_j^{\dagger}\underbrace{\left\{1 - \frac{1}{2S}a_j^{\dagger}a_j\right\}^{1/2}}_{f(a_j^{\dagger}a_j)}$$

Pero, **se mantienen las relaciones de conmutación del momento angular**

$$\Rightarrow [S_j^+, S_j^-] = 2S\left(f(a_j^{\dagger}a_j)a_j a_j^{\dagger} f(a_j^{\dagger}a_j) - a_j^{\dagger} f^2(a_j^{\dagger}a_j)a_j\right)$$
$$= 2(S - a_j^{\dagger}a_j)$$

$$\rightarrow S_j^z = S - a_j^{\dagger}a_j$$

Determina la desviación de S respecto al operador n° de ocupación (N° de excitaciones)

Ondas de espín

6.3 Spin Waves in Ferromagnets

Transformación de Holstein-Primakoff ⟶ Representación en número de ocupación

¿Cuánto se desvía S_j^z de su valor máximo S?

Consideramos nuevamente el régimen de bajas temperaturas ⟶ $\langle a_j^\dagger a_j \rangle \ll S$
(low-energy excitations)

Esto nos permite expandir $f(a_j^\dagger a_j)$
de modo que:

$$S_j^+ = \sqrt{2S}\Big\{1 - \frac{1}{4S} a_j^\dagger a_j + \dots\Big\} a_j \simeq \sqrt{2S} a_j, \text{ and } S_j^- \simeq \sqrt{2S} a_j^\dagger$$

$$\begin{aligned}
\Rightarrow \quad \mathcal{H}_{\text{spin}} &\simeq -J \sum_{n.n.i,j} \Big\{ S(a_i a_j^\dagger + a_i^\dagger a_j) + S^2 - S(a_i a_i^\dagger + a_j^\dagger a_j) \Big\} \\
&\simeq -E_0 + JS \sum_{n.n.i,j} \Big\{ a_i^\dagger a_i + a_j^\dagger a_j - a_i a_j^\dagger - a_i^\dagger a_j \Big\}
\end{aligned}$$

Ondas de espín

6.3 Spin Waves in Ferromagnets

Transformación de Holstein-Primakoff

$$\mathcal{H}_{\text{spin}} \simeq -J \sum_{n.n.i,j} \left\{ S(a_i a_j^\dagger + a_i^\dagger a_j) + S^2 - S(a_i a_i^\dagger + a_j^\dagger a_j) \right\}$$

$$\simeq -E_0 + JS \sum_{n.n.i,j} \left\{ a_i^\dagger a_i + a_j^\dagger a_j - a_i a_j^\dagger - a_i^\dagger a_j \right\}$$

→ Interacciones entre sitios vecinos

Cambio de representación → $a_j = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} b_{\boldsymbol{k}}, \quad a_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} b_{\boldsymbol{k}}^\dagger$

1) $$\sum_{n.n.ij} a_j^\dagger a_j = \nu \sum_{\boldsymbol{k}\boldsymbol{k}'} \underbrace{\frac{1}{N} \sum_j \mathrm{e}^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_j}}_{\delta_{\boldsymbol{k}\boldsymbol{k}'}} b_{\boldsymbol{k}'}^\dagger b_{\boldsymbol{k}} = \nu \sum_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}}$$

2) $$\sum_{n.n.ij} a_i^\dagger a_j = \sum_{\boldsymbol{k}\boldsymbol{k}'} \frac{1}{N} \sum_{n.n.ij} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}_j} b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}'}$$

$$= \sum_{\boldsymbol{k}\boldsymbol{k}'} \frac{1}{N} \sum_j \mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_j} \sum_{\boldsymbol{d}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}} b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}'} = \nu \sum_{\boldsymbol{k}} \gamma_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}}$$

Ondas de espín

6.3 Spin Waves in Ferromagnets

Transformación de Holstein-Primakoff

$$\mathcal{H}_{\text{spin}} \simeq -J \sum_{n.n.i,j} \left\{ S(a_i a_j^\dagger + a_i^\dagger a_j) + S^2 - S(a_i a_i^\dagger + a_j^\dagger a_j) \right\}$$

$$\simeq -E_0 + JS \sum_{n.n.i,j} \left\{ a_i^\dagger a_i + a_j^\dagger a_j - a_i a_j^\dagger - a_i^\dagger a_j \right\}$$

→ Interacciones entre sitios vecinos

Cambio de representación → $a_j = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_j} b_{\boldsymbol{k}}, \quad a_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_j} b_{\boldsymbol{k}}^\dagger$

$$\mathcal{H}_{\text{spin}} \simeq E_0 + 2J\nu S \sum_{\boldsymbol{k}} (1 - \gamma_{\boldsymbol{k}}) b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}} = E_0 + \sum_{\boldsymbol{k}} \hbar\omega_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}}$$

Hamiltoniano para ondas de espín en ferromagnets

$$\sum_j S_j^z = NS - \sum_{\boldsymbol{k}} b_{\boldsymbol{k}}^\dagger b_{\boldsymbol{k}}$$

Excitaciones colectivas – MAGNONES

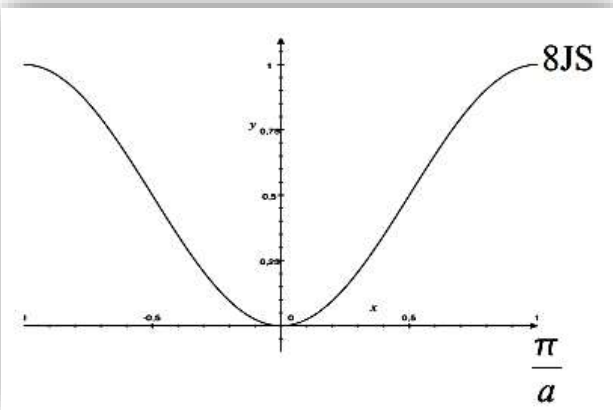
Ondas de espín

6.3 Spin Waves in Ferromagnets

Contribución de Magnones al calor específico

$$\gamma_{\mathbf{k}} = \frac{1}{\nu}\sum_{\mathbf{d}} e^{i\mathbf{k}\cdot\mathbf{d}}$$

Para $k \ll \pi/a$ se puede aproximar → $1-\gamma_{\mathbf{k}} \simeq 1-(1-\frac{1}{2\nu}\sum_{\mathbf{d}}|\mathbf{k}\cdot\mathbf{d}|^2) \sim k^2$



Relación de dispersión en 1D:

$$\hbar\omega = 4J|S|(1-\cos(ka))$$

$$E(T) = E_0 + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}\langle b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}\rangle$$

→ Distribución de Bose-Einstein

$$= E_0 + \frac{V}{(2\pi)^3}\int \hbar\omega_{\mathbf{k}} \frac{1}{e^{\beta\hbar\omega_{\mathbf{k}}}-1} d^3k.$$

$$= E_0 + \frac{\alpha}{2\pi^2}\left(\frac{k_B T}{\alpha}\right)^{5/2}\int_0^{x_{max}} x^{3/2}\frac{1}{e^x-1}dx.$$

$[x = \beta\alpha k^2]$

$T \approx 0K,\ \hbar\omega_{\mathbf{k}} = \alpha k^2 \rightarrow \alpha = 2JSa^2$

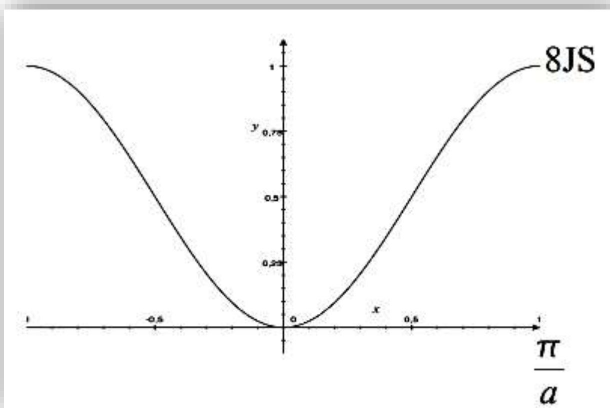
Ondas de espín

6.3 Spin Waves in Ferromagnets

Contribución de Magnones al calor específico

$$\gamma_{\boldsymbol{k}} = \frac{1}{\nu} \sum_{\boldsymbol{d}} e^{i\boldsymbol{k}\cdot\boldsymbol{d}}$$

Para $k \ll \pi/a$ se puede aproximar → $1 - \gamma_{\boldsymbol{k}} \simeq 1 - \left(1 - \frac{1}{2\nu}\sum_{\boldsymbol{d}} |\boldsymbol{k}\cdot\boldsymbol{d}|^2\right) \sim k^2$



Relación de dispersión en 1D:

$$\hbar\omega = 4J\,|S|\left(1 - \cos(ka)\right)$$

$$E(T) = E_0 + \sum_{\boldsymbol{k}} \hbar\omega_{\boldsymbol{k}} \langle b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}} \rangle$$

→ Distribución de Bose-Einstein

$$= E_0 + \frac{V}{(2\pi)^3} \int \hbar\omega_{\boldsymbol{k}} \frac{1}{e^{\beta\hbar\omega_{\boldsymbol{k}}} - 1} d^3k.$$

$$= E_0 + \frac{\alpha}{2\pi^2} \left(\frac{k_B T}{\alpha}\right)^{5/2} \int_0^{x_{\max}} x^{3/2} \frac{1}{e^x - 1} dx.$$

$T \approx 0K \xrightarrow{x_{max} \to \infty} E(T) = E_0 + \frac{0.45}{\pi^2 \alpha^{3/2}} (k_B T)^{5/2}$

$$c_V(T) = \left.\frac{dE(T)}{dT}\right|_{V=\text{const.}} = 0.113\, k_B \left(\frac{k_B T}{\alpha}\right)^{3/2}$$

Ondas de espín

6.4 Spin Waves in Anti-Ferromagnets

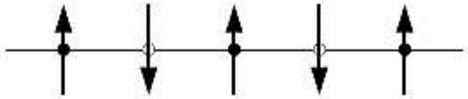


Fig. 6.6. Linear chain with anti-ferromagnetic order, the Wigner–Seitz cell contains two ions with opposite spin

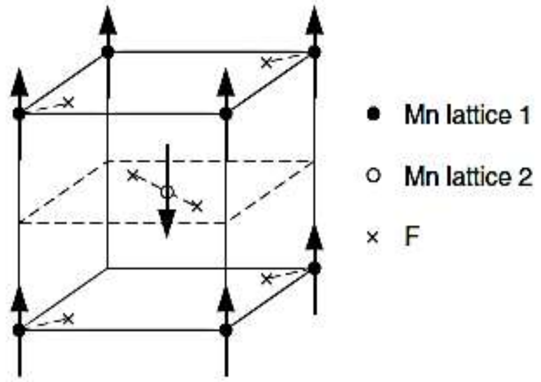


Fig. 6.7. Structure of the anti-ferromagnetic insulator MnF_2

$$\mathcal{H}_{\text{spin}} = J_a \sum_{n.n.i,j} \boldsymbol{S}_{1i} \cdot \boldsymbol{S}_{2j} = J_a \sum_{n.n.ij} \left(\frac{1}{2} \left(S_{1i}^{+} S_{2j}^{-} + S_{1i}^{-} S_{2j}^{+} \right) + S_{1i}^{z} S_{2j}^{z} \right)$$

$J_a > 0$

Ondas de espín

6.4 Spin Waves in Anti-Ferromagnets

$$\mathcal{H}_{\text{spin}} = J_a \sum_{n.n.i,j} \boldsymbol{S}_{1i} \cdot \boldsymbol{S}_{2j} = J_a \sum_{n.n.ij} \left(\frac{1}{2}(S_{1i}^+ S_{2j}^- + S_{1i}^- S_{2j}^+) + S_{1i}^z S_{2j}^z \right)$$

Transformación de Holstein-Primakoff

$$\begin{cases} S_{1i}^+ \simeq \sqrt{2S} a_{1i},\ S_{1i}^- \simeq \sqrt{2S} a_{1i}^\dagger,\ S_{1i}^z = +S - a_{1i}^\dagger a_{1i} \quad \text{(sublattice 1)} \\ S_{2i}^+ \simeq \sqrt{2S} a_{2i},\ S_{2i}^- \simeq \sqrt{2S} a_{2i}^\dagger,\ S_{2i}^z = -S + a_{2i}^\dagger a_{2i} \quad \text{(sublattice 2)} \end{cases}$$

Low-energy excitations → $\langle a_{1i}^\dagger a_{1i} \rangle, \langle a_{2i}^\dagger a_{2i} \rangle \ll S$

$$\mathcal{H}_{\text{spin}} \simeq J_a \sum_{n.n.ij} \{ -S^2 + S(a_{1i}^\dagger a_{1i} + a_{2i}^\dagger a_{2i} + a_{1i} a_{2j} + a_{1i}^\dagger a_{2j}^\dagger) \}$$

$$a_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} b_{\boldsymbol{k}}^\dagger$$

$$a_j = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_j} b_{\boldsymbol{k}}$$

$$\mathcal{H}_{\text{spin}} \simeq E_a + 2J_a \nu S \sum_{\boldsymbol{k}} \left\{ b_{1\boldsymbol{k}}^\dagger b_{1\boldsymbol{k}} + b_{2\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}} + \gamma_{\boldsymbol{k}} (b_{1\boldsymbol{k}}^\dagger b_{2\boldsymbol{k}}^\dagger + b_{1\boldsymbol{k}} b_{2\boldsymbol{k}}) \right\}$$

$E_a = -2J_a \nu N S^2$ ¿Energía del estado fundamental?

Ondas de espín

6.4 Spin Waves in Anti-Ferromagnets

$$\mathcal{H}_{\text{spin}} \simeq E_a + 2J_a\nu S \sum_{\boldsymbol{k}} \left\{ \underbrace{b^\dagger_{1\boldsymbol{k}} b_{1\boldsymbol{k}} + b^\dagger_{2\boldsymbol{k}} b_{2\boldsymbol{k}}}_{\text{Excitaciones en cada sublattice}} + \gamma_{\boldsymbol{k}} \underbrace{\left(b^\dagger_{1\boldsymbol{k}} b^\dagger_{2\boldsymbol{k}} + b_{1\boldsymbol{k}} b_{2\boldsymbol{k}} \right)}_{\text{Acoplamientos entre sublattices}} \right\}$$

Transformación de Bogoliubov

$$\begin{cases} \alpha_{\boldsymbol{k}} = u_{\boldsymbol{k}} b_{1\boldsymbol{k}} - v_{\boldsymbol{k}} b^\dagger_{2\boldsymbol{k}}, & \alpha^\dagger_{\boldsymbol{k}} = u_{\boldsymbol{k}} b^\dagger_{1\boldsymbol{k}} - v_{\boldsymbol{k}} b_{2\boldsymbol{k}} \\ \beta_{\boldsymbol{k}} = u_{\boldsymbol{k}} b_{2\boldsymbol{k}} - v_{\boldsymbol{k}} b^\dagger_{1\boldsymbol{k}}, & \beta^\dagger_{\boldsymbol{k}} = u_{\boldsymbol{k}} b^\dagger_{2\boldsymbol{k}} - v_{\boldsymbol{k}} b_{1\boldsymbol{k}} \end{cases}$$

→ $u_{\boldsymbol{k}}$, $v_{\boldsymbol{k}}$ son coeficientes reales

→ Los nuevos operadores cumplen las reglas de conmutación de bosones

$$[\alpha_{\boldsymbol{k}}, \alpha^\dagger_{\boldsymbol{k}'}] = [\beta_{\boldsymbol{k}}, \beta^\dagger_{\boldsymbol{k}'}] = \delta_{\boldsymbol{k}\boldsymbol{k}'}, \; [\alpha_{\boldsymbol{k}}, \beta_{\boldsymbol{k}'}] = [\alpha^\dagger_{\boldsymbol{k}}, \beta^\dagger_{\boldsymbol{k}'}] = [\alpha_{\boldsymbol{k}}, \beta^\dagger_{\boldsymbol{k}'}] = 0 \longrightarrow u^2_{\boldsymbol{k}} - v^2_{\boldsymbol{k}} = 1$$

$$b_{1\boldsymbol{k}} = u_{\boldsymbol{k}} \alpha_{\boldsymbol{k}} + v_{\boldsymbol{k}} \beta^\dagger_{\boldsymbol{k}}, \; b_{2\boldsymbol{k}} = u_{\boldsymbol{k}} \beta_{\boldsymbol{k}} + v_{\boldsymbol{k}} \alpha^\dagger_{\boldsymbol{k}}$$

Reemplazamos en $\mathcal{H}_{\text{spin}}$

Ondas de espín

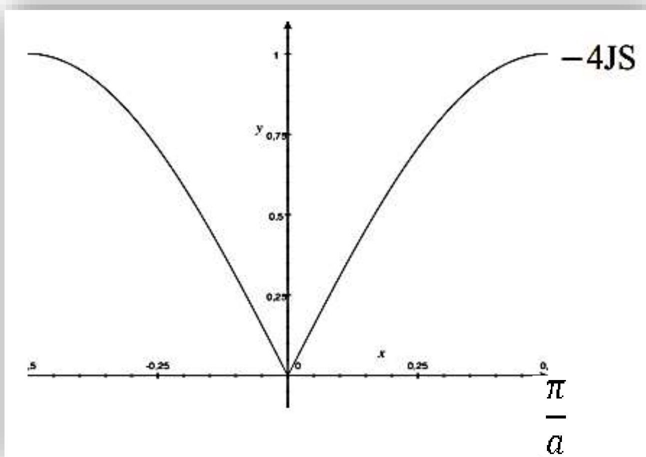
6.4 Spin Waves in Anti-Ferromagnets

$$\mathcal{H}_{\text{spin}} = -2J_a\nu NS(S+1) + \sum_{\boldsymbol{k}} \hbar\omega_{\boldsymbol{k}}(\alpha_{\boldsymbol{k}}^{\dagger}\alpha_{\boldsymbol{k}} + \beta_{\boldsymbol{k}}^{\dagger}\beta_{\boldsymbol{k}} + 1)$$

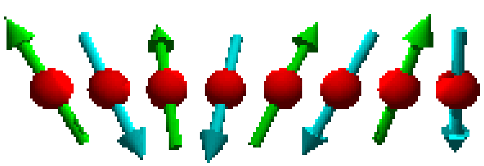
Hamiltoniano para ondas de espín en anti-ferromagnets

Relación de dispersión → $\hbar\omega_{\boldsymbol{k}} = 2J_a\nu S(1-\gamma_{\boldsymbol{k}}^2)^{1/2}$

Para $k \ll \pi/a$ → $1-\gamma_{\boldsymbol{k}}^2 \sim k^2$



⇒ $\hbar\omega_{\boldsymbol{k}} \sim k$



Ondas de espín

6.4 Spin Waves in Anti-Ferromagnets

$$\mathcal{H}_{\text{spin}} = -2J_a \nu N S(S+1) + \sum_{\boldsymbol{k}} \hbar\omega_{\boldsymbol{k}} (\alpha^\dagger_{\boldsymbol{k}} \alpha_{\boldsymbol{k}} + \beta^\dagger_{\boldsymbol{k}} \beta_{\boldsymbol{k}} + 1)$$

Hamiltoniano para ondas de espín en anti-ferromagnets

Energía del estado fundamental

$$E_0 = \langle \Psi_0 | \mathcal{H}_{\text{spin}} | \Psi_0 \rangle = -2J_a \nu N S^2 - 2J_a \nu S \sum_{\boldsymbol{k}} \left(1 - \sqrt{1-\gamma^2_{\boldsymbol{k}}}\right)$$

Energía de la configuración antiferromagnética

Zero-point contribution (desviación de E_a)

Thus, in the ground state, the magnon vacuum, the spins in the individual sublattices are not perfectly aligned but slightly disordered.

¡Muchas gracias!