Spin Waves and Electronic Interactions in La_2CuO_4

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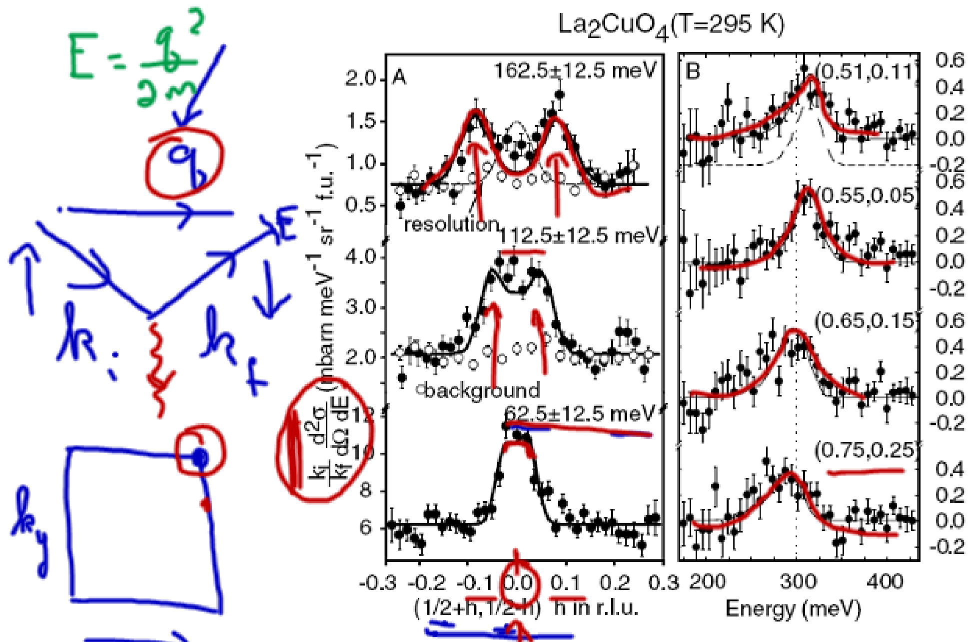
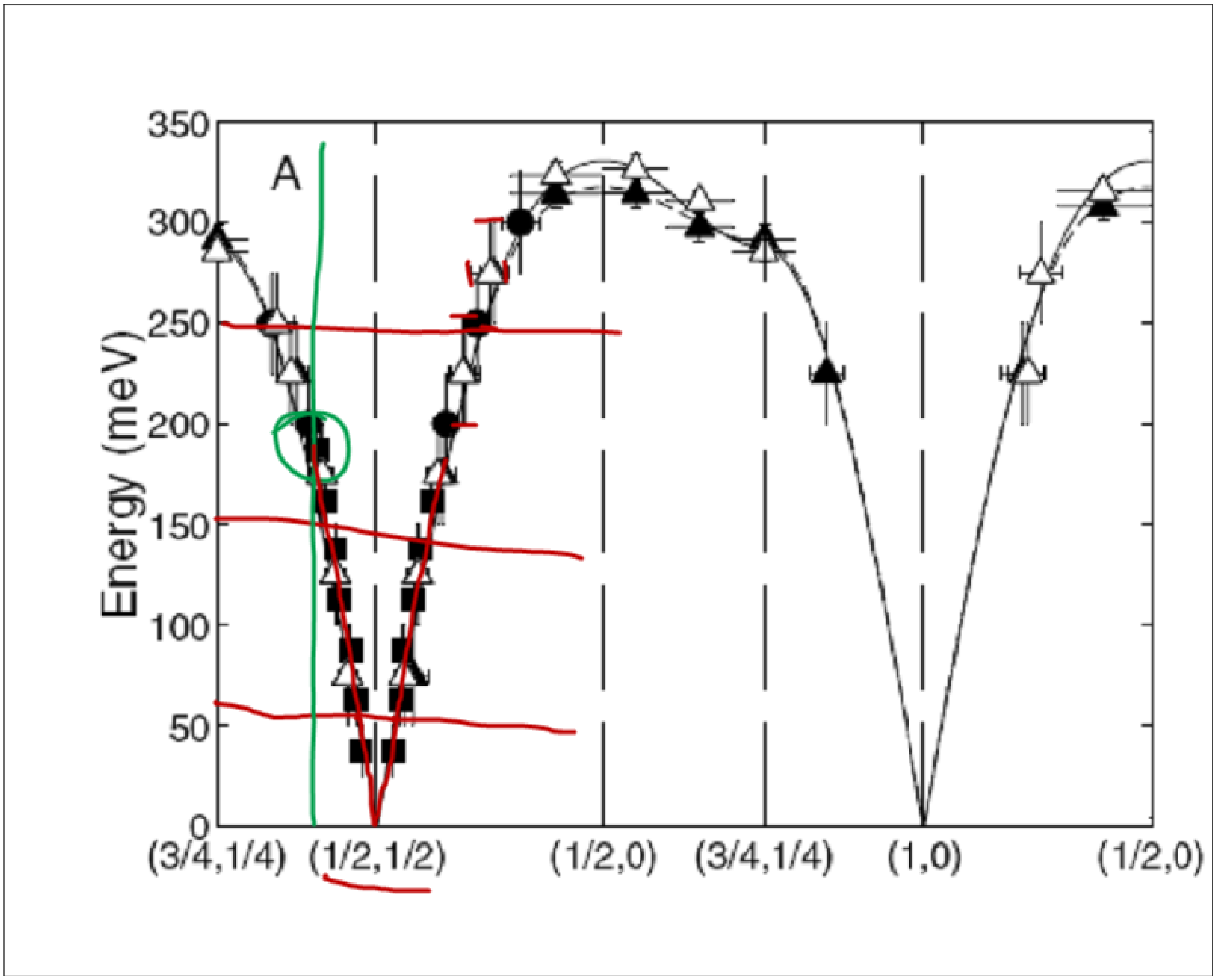


FIG. 2. Scattering from the spin waves in La_2CuO_4 (T = 295 K). Data result from 68 h (A) and 98 h (B) counting at a proton current of 170 μA. The sample is described in [10]. Solid lines are fits to a spin-wave cross section convolved with the instrumental resolution. (A) Const-E cuts near the AF zone center for an incident energy E_i = 250 meV. Q_z wave vector components at scan centers are l = 2.8 (bottom panel), 6.2, and 9.6 r.l.u. of 0.477 $Å^{-1}$. Open circles are a background measured near the (0, 0) position. Dashed curve is the instrumental response to spin waves of infinite velocity. (B) Const-Q cuts, with E_i = 750 meV, yield the dispersion along the AF zone boundary. Vertical dotted line at E = 300 meV is a guide to the eye. l values at peak position vary from 8.8 (bottom panel) to 9.5 (top panel). A background measured near the nuclear zone center (1, 0) has been subtracted. Dashed curve is the instrumental response to a dispersionless mode.



A
Energy (meV)
350
300
250
200
150
100
50
0
(3/4,1/4)
(1/2,1/2)
(1/2,0)
(3/4,1/4)
(1,0)
(1/2,0)

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$H_{int} =$

$i=j \quad k=l \rightarrow 0$

$i=j=k \quad l \rightarrow 0$

$$\frac{1}{2}\sum_{\substack{ijkl \\ \sigma\sigma'}} \underbrace{\langle i\sigma| \langle j\sigma'| V |k\sigma\rangle |l\sigma'\rangle}_{} \; c^{+}_{i\sigma} c^{+}_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

$$= \int d^3r\, d^3r'\, V(\vec{r}-\vec{r}')\, w^*(\vec{r}-\vec{R}_i)\, w^*(\vec{r}'-\vec{R}_j)\, w(\vec{r}-\vec{R}_k)\, w(\vec{r}'-\vec{R}_l)$$

Hubbard

$i=j=k=l$

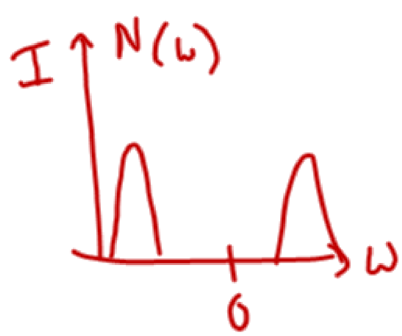
$$\boxed{H_{int} = U\sum_i n_{i\uparrow} n_{i\downarrow}}$$

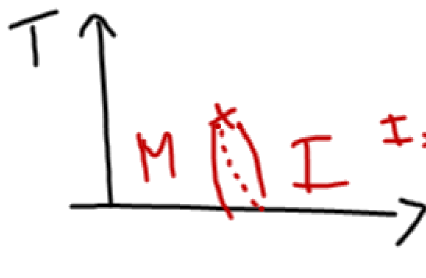
$\vec{R}_j$

2^{N} dég.

$$\sum_{ij\sigma} t_{ij}\, c^{+}_{i\sigma} c_{j\sigma}$$

$$\boxed{U \gg t}$$





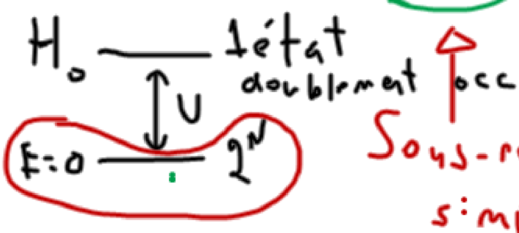
$d=\infty$

Isolat de Mott

Modèle de Heisenberg Ferromagnétique

Diagonaliser V dans le sous-espace des 2^N états ayant 1 électron par site

$$|\Psi\rangle = |\alpha\rangle + \sum_{m \neq \alpha} \frac{|m\rangle\langle m|H_1|\alpha\rangle}{E_\alpha - E_m} + \dots$$



Sous-espace simplement occupé

H_1 = pert.

$$\langle \Psi' | H_0 + H_1 | \Psi \rangle$$ à diagonaliser

$$\frac{1}{2}\sum_{\substack{ijkl\\ \sigma\sigma'}} \langle i\sigma|\langle j\sigma'|V|k\sigma\rangle|l\sigma'\rangle \quad c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

$$= \sum_{\substack{ij\\ \sigma\sigma'}} \int d^3r\, d^3r'\, \frac{1}{2} V(\vec r - \vec r')\, w^*(\vec r - \vec R_i)\, w(\vec r' - \vec R_i)\, w^*(\vec r - \vec R_j)\, w(\vec r' - \vec R_j)$$

$$c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} c_{j\sigma}$$

$$= \sum_{\substack{ij\\ \sigma\sigma'}} \left(-\frac{J_{ij}}{2}\right) c^\dagger_{i\sigma} c_{i\sigma'}\, c^\dagger_{j\sigma'} c_{j\sigma}$$

$$\sigma = \sigma' : \quad c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\uparrow}$$

$$+ c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{j\downarrow} c_{j\downarrow} = n_{i\uparrow} n_{j\uparrow} + n_{i\downarrow} n_{j\downarrow}$$

$$= \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow})(n_{j\uparrow} + n_{j\downarrow})$$

$$+ \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow})$$

$$= \frac{1}{2}\left(\frac{2}{\hbar} S^z_i \quad \frac{2}{\hbar} S^z_j\right)$$

$$-\frac{J_{ij}}{\hbar^2}\, 2\, S^z_i S^z_j$$

$$\sigma = -\sigma' : \quad c^\dagger_{i\uparrow} c_{i\downarrow} c^\dagger_{j\downarrow} c_{j\uparrow}$$

$$+ c^\dagger_{i\downarrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\downarrow}$$

$$= \frac{1}{\hbar^2}\left(S^+_i S^-_j + S^-_i S^+_j\right)$$

$$\sum_{ij} \frac{-2J_{ij}}{\hbar^2}\, \frac{1}{2}\left[S^z_i S^z_j + \frac{1}{2}\left(S^+_i S^-_j + S^-_i S^+_j\right)\right]$$

$$= \boxed{\sum_{ij}\left(-\frac{J_{ij}}{\hbar^2}\right) \vec S_i \cdot \vec S_j}$$

Heisenberg ferro

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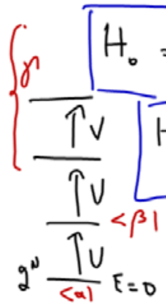
Super-échange: (effet de t_{ij})

Théorie des perturbations dégénérées.



$$H_0 = U\sum_i n_{i\uparrow} n_{i\downarrow}$$

$$H_1 = -t\sum_{\langle ij\rangle}\left(c^+_{i\sigma}c_{j\sigma} + c^+_{j\sigma}c_{i\sigma}\right)$$

$$t_{ij} = \langle i\sigma|-\frac{\hbar^2}{2m}\nabla^2 - V|j\sigma\rangle$$

$\langle ij\rangle$ chaque lien compté 1 fois

(ij) chaque lien compté 2 fois

$$\boxed{|\Psi\rangle = |\alpha\rangle + \sum_{m\neq\alpha}\frac{|m\rangle\langle m|H_1|\alpha\rangle}{E_\alpha - E_m} + \dots}$$

à l'ordre dominant:

$$\langle\alpha'|H_0+H_1|\alpha\rangle = 0 +$$

À l'ordre suivant

$$|\Psi\rangle = |\alpha\rangle + \sum_\beta \frac{|\beta\rangle\langle\beta|H_1|\alpha\rangle}{-U}$$

$$= |\alpha\rangle - \frac{1}{U}\sum_m |m\rangle\langle m|H_1|\alpha\rangle$$

$$= |\alpha\rangle - \frac{1}{U}H_1|\alpha\rangle$$

$$\left(\langle\alpha'| - \frac{1}{U}\langle\alpha'|H_1\right)\left(H_0+H_1\right)\left(|\alpha\rangle - \frac{1}{U}H_1|\alpha\rangle\right)$$

$$-\langle\alpha'|H_1\frac{1}{U}H_1|\alpha\rangle \quad (1)$$

$$-\frac{1}{U}\langle\alpha'|H_1\,H_0\left(|\alpha\rangle - \frac{1}{U}H_1|\alpha\rangle\right) \quad 0 \quad (3)$$

$$-\frac{1}{U}\langle\alpha'|H_1H_1\left(|\alpha\rangle - \cancel{\frac{1}{U}H_1|\alpha\rangle}\right) \quad (1)$$

$$= -\frac{2}{U}\langle\alpha'|H_1H_1|\alpha\rangle \quad (1)$$

$$+\frac{1}{U^2}\langle\alpha'|H_1H_0H_1|\alpha\rangle \quad (3)$$

$$-\frac{1}{U}\langle\alpha'|\underbrace{H_1 H_1}|\alpha\rangle$$

à diagonaliser

$$\underbrace{H_1 H_1} = t^2 \sum_{\substack{\langle ij\rangle \\ \sigma}} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma})$$

$$\sum_{\substack{\langle kl\rangle \\ \sigma'}} (c^\dagger_{k\sigma'} c_{l\sigma'} + c^\dagger_{l\sigma'} c_{k\sigma'})$$

$$= t^2 \sum_{\substack{\langle ij\rangle \\ \sigma\sigma'}} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma})(c^\dagger_{i\sigma'} c_{j\sigma'} + c^\dagger_{j\sigma'} c_{i\sigma'})$$

$$= 2t^2 \sum_{\substack{\langle ij\rangle \\ \sigma\sigma'}} c^\dagger_{i\sigma} c_{j\sigma} c^\dagger_{j\sigma'} c_{i\sigma'}$$

$$= 2t^2 \sum_{\substack{\langle ij\rangle \\ \sigma\sigma'}} c^\dagger_{i\sigma} c_{i\sigma'} c_{j\sigma} c^\dagger_{j\sigma'}$$

$$c_{j\sigma} c^\dagger_{j\sigma'} = \delta_{\sigma\sigma'} - \underbrace{c^\dagger_{j\sigma'} c_{j\sigma}}$$

Contribution

$$2t^2 \sum_{\substack{\langle ij\rangle \\ \sigma}} c^\dagger_{i\sigma} c_{i\sigma}$$

à cte près :

$$\boxed{= -2t^2 \sum_{\substack{\langle ij\rangle \\ \sigma\sigma'}} \underbrace{c^\dagger_{i\sigma} c_{i\sigma'}}\ \underbrace{c^\dagger_{j\sigma'} c_{j\sigma}}}$$

$$\langle\alpha'|\frac{H_1 H_1}{U}|\alpha\rangle = \langle\alpha'|\frac{2t^2}{U}\frac{2}{\hbar^2}\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j |\alpha\rangle$$

$$= \langle\alpha'| \frac{4t^2}{U\hbar^2} \sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j |\alpha\rangle$$

$$= \boxed{\langle\alpha'| J \sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j |\alpha\rangle}$$

$$\boxed{J = \frac{4t^2}{U\hbar^2}}.$$

S est grand

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Chapitre 6

Modes collectifs, ondes de spin

Cas ferromagnétique:

$-|J| \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$ Fondamental:

$|\uparrow\uparrow\uparrow\uparrow\uparrow \ldots\rangle$

États excités? Ferromagnétique $\uparrow\downarrow$

Essai: $|\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$

$\downarrow\uparrow$

$$|\uparrow\uparrow\uparrow\underset{1}{\overset{i}{\downarrow}}\uparrow\uparrow\uparrow\rangle \frac{1}{\sqrt{N}} e^{ikr_i}$$

$$+ |\uparrow\uparrow\underset{2}{\downarrow}\uparrow\uparrow\uparrow\uparrow\rangle \frac{1}{\sqrt{N}} e^{ikr_{i-1}}$$

$$+ |\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle \frac{1}{\sqrt{N}} e^{ikr_{i-2}}$$

$\vdots$

Définition

$$S_i^z = S - a_i^+ a_i$$

$$S_i^+ = \sqrt{2S - a_i^+ a_i}\, a_i$$

$$S_i^- = a_i^+ \sqrt{2S - a_i^+ a_i}$$

$$S_- |m\rangle = \sqrt{2m}\, |S-1\rangle$$

où

$$[a_i, a_j^+] = \delta_{ij}$$

$$[S_i^+, S_j^-] = 2 S_i^z \delta_{ij}$$

$$[S_i^z, S_j^\pm] = \pm S_i^\pm \delta_{ij}$$

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