Magnetism

We saw in the slides

$$H = J \sum_{\langle ij \rangle} S_i \cdot S_j$$

but where does this Hamiltonian come from?

I'll use a toy example to motivate this.

You can also see books by Fazekas and Girvin + Yang

Also: handwritten notes are available at

sites.google.com/site/hiteshchanglani/teaching

What is the origin of magnetism?

I $\quad \underset{a}{\uparrow} \;\; \underset{b}{\uparrow}$ $\qquad$ II $\quad \underset{a}{\uparrow} \;\; \underset{b}{\downarrow}$ $\qquad$ III $\quad \underset{a}{\downarrow} \;\; \underset{b}{\uparrow}$ $\qquad$ IV $\quad \underset{a}{\downarrow} \;\; \underset{b}{\downarrow}$

$$H = \underbrace{h_0(r_1)}_{-\frac{\hbar^2}{2m}\nabla_1^2 + V(r_1)} + \underbrace{h_0(r_2)}_{-\frac{\hbar^2}{2m}\nabla_2^2 + V(r_2)} + \underbrace{\frac{e^2}{|r_1 - r_2|}}$$

electrons are fermions $\longrightarrow$ wf antisymmetric

$r_1, s_1, r_2, s_2 \ldots$

$$\left.\begin{aligned} h_0(r)\,\varphi_a(r) &= \varepsilon_a\,\varphi_a(r) \\ h_0(r)\,\varphi_b(r) &= \varepsilon_b\,\varphi_b(r) \end{aligned}\right\}$$

$$\int \varphi_a^* \varphi_b \, d^3r = 0$$

$$\psi_1(r_1, s_1, r_2, s_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_a(r_1)\,\alpha(s_1) & \varphi_a(r_2)\,\alpha(s_2) \\ \varphi_b(r_1)\,\alpha(s_1) & \varphi_b(r_2)\,\alpha(s_2) \end{vmatrix}$$

$\uparrow$ determinant

✓

$$\psi_4 = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_a(r_1)\,\beta(s_1) & \varphi_a(r_2)\,\beta(s_2) \\ \varphi_b(r_1)\,\beta(s_1) & \varphi_b(r_2)\,\beta(s_2) \end{vmatrix}$$

$$\psi_2 = \frac{1}{\sqrt{2}} \begin{vmatrix} \varphi_a(r_1)\,\alpha(s_1) & \varphi_a(r_2)\,\alpha(s_2) \\ \varphi_b(r_1)\,\beta(s_1) & \varphi_b(r_2)\,\beta(s_2) \end{vmatrix}$$

ψ_3 = similar to ψ_2

$\langle \psi_i | H | \psi_j \rangle \qquad i,j = 1,2,3,4 \quad \rightarrow \quad 4 \times 4$ matrix

$\Downarrow$ diagonalize this! Corresponds to solving TIDSE

$$\langle \psi_i | \underbrace{h_0(r_1) + h_0(r_2) + \frac{e^2}{|r_1 - r_2|}}_{\text{Kinetic + Coulomb}} | \psi_j \rangle$$

$$\langle \psi_1 | h_0(r_1) | \psi_1 \rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \int \sum_{s_1, s_2} \alpha^*(s_1)\,\alpha^*(s_2) \left[\varphi_a^*(r_1)\,\varphi_b^*(r_2) - \varphi_a^*(r_2)\,\varphi_b^*(r_1)\right]$$

$$h_0(r_1) \left[\varphi_a(r_1)\,\varphi_b(r_2) - \varphi_a(r_2)\,\varphi_b(r_1)\right]$$

$\alpha(s_1)\,\alpha(s_2) \quad d^3r$

$$= \frac{\varepsilon_a + \varepsilon_b}{2}$$

$\langle \psi_i | \, h_0(r_1) + h_0(r_2) \, | \psi_j \rangle \rightarrow 4 \times 4$ matrix

$$\varepsilon_a + \varepsilon_b \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\frac{e^2}{|r_1 - r_2|}$$

$$\begin{aligned}
\langle \psi_1 | \frac{e^2}{|r_1 - r_2|} | \psi_1 \rangle = {} & \frac{1}{2} \int \frac{|\varphi_a(r_1)|^2 |\varphi_b(r_2)|^2 e^2}{|r_1 - r_2|} \, d^3r_1 \, d^3r_2 \\
& + \frac{1}{2} \int \frac{|\varphi_a(r_2)|^2 |\varphi_b(r_1)|^2 e^2}{|r_1 - r_2|} \, d^3r_1 \, d^3r_2 \quad r_1 \leftrightarrow r_2 \\
& - \frac{1}{2} \int \frac{\varphi_a^*(r_1)\varphi_a(r_2)\varphi_b^*(r_2)\varphi_b(r_1) \, e^2}{|r_1 - r_2|} \, d^3r_1 \, d^3r_2 \\
& - \frac{1}{2} \int \frac{\varphi_a^*(r_2)\varphi_a(r_1)\varphi_b^*(r_1)\varphi_b(r_2) \, e^2}{|r_1 - r_2|} \, d^3r_1 \, d^3r_2
\end{aligned}$$

$$= C_{ab} - J_{ab}$$

> 0

$$H = \underbrace{\varepsilon_a + \varepsilon_b \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{\text{diagonal ✓}} + \underbrace{\begin{pmatrix} \boxed{C_{ab} - J_{ab}} & 0 & 0 & 0 \\ 0 & C_{ab} & -J_{ab} & 0 \\ 0 & -J_{ab} & C_{ab} & 0 \\ 0 & 0 & 0 & \boxed{C_{ab} - J_{ab}} \end{pmatrix}}$$

✓

$$\underbrace{\varphi_a(r_1)\,\varphi_b(r_1)}_{<0} \qquad \underbrace{\varphi_a(r_2)\,\varphi_b(r_2)}_{<0}$$

$r_2 \simeq r_1$

$C_{ab} > 0$

$J_{ab} > 0$

$\Psi_1 \quad \underset{a}{\uparrow} \quad \underset{b}{\uparrow}$ $\qquad \varepsilon = \varepsilon_a + \varepsilon_b + C_{ab} - J_{ab}$

$\Psi_4 \quad \underset{a}{\downarrow} \quad \underset{b}{\downarrow}$ $\qquad \varepsilon = \varepsilon_a + \varepsilon_b + C_{ab} - J_{ab}$

$$\begin{array}{c|c} & \begin{array}{cc} |\Psi_2\rangle & |\Psi_3\rangle \end{array} \\ \begin{array}{c} \langle\Psi_2| \\ \langle\Psi_3| \end{array} & \begin{pmatrix} C_{ab} & -J_{ab} \\ -J_{ab} & C_{ab} \end{pmatrix} \end{array}$$

$$(C_{ab} - \varepsilon)^2 - J_{ab}^2 = 0$$

$$C_{ab} - \varepsilon = \pm J_{ab}$$

$$\mathcal{E} = \varepsilon_a + \varepsilon_b + (C_{ab} - J_{ab})$$

$$\mathcal{E} = \varepsilon_a + \varepsilon_b + (C_{ab} + J_{ab})$$

$$- \quad \varepsilon_a + \varepsilon_b + C_{ab} + J_{ab} \qquad \frac{\uparrow\downarrow - \downarrow\uparrow}{\sqrt{2}}$$

$$\uparrow\uparrow \quad \downarrow\downarrow \quad \frac{\uparrow\downarrow + \downarrow\uparrow}{\sqrt{2}} \qquad \varepsilon_a + \varepsilon_b + C_{ab} - J_{ab}$$

$s \;\; m_s$

$$|1,1\rangle = |\psi_1\rangle$$

$$|1,-1\rangle = |\psi_4\rangle$$

$$|1,0\rangle = \frac{|\psi_2\rangle + |\psi_3\rangle}{\sqrt{2}}$$

"Triplet"

$$|0,0\rangle = \frac{|\psi_2\rangle - |\psi_3\rangle}{\sqrt{2}}$$

"Singlet"

$$S^2 |s, m_s\rangle = s(s+1)|s, m_s\rangle$$

Triplet:

$$S^2 |1, m_s\rangle = 1(1+1)|1, m_s\rangle = 2|1, m_s\rangle$$

$$|0,0\rangle = 0(0+1)|0,0\rangle = 0|0,0\rangle$$

$$S^2 - 1 \,|\,\rangle = 1 \,|1, m_s\rangle \quad \text{Triplet}$$

$$|\,\rangle \quad -1 \,|0,0\rangle \quad \text{Singlet}$$

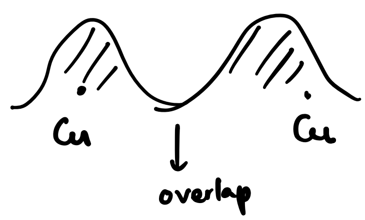
$$\mathcal{E} = \varepsilon_a + \varepsilon_b + C_{ab} - J_{ab}\,\underbrace{(S^2 - 1)}$$

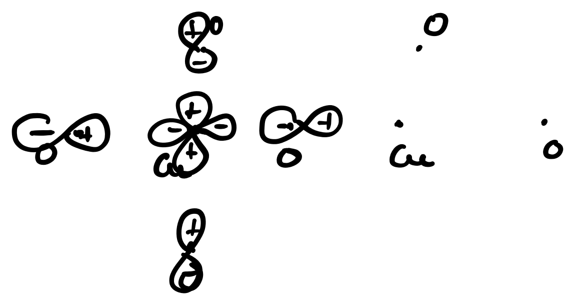
$$S^2 = (S_1 + S_2)^2 = S_1^2 + S_2^2 + 2\, S_1 \cdot S_2$$

$$\mathcal{E} = \underbrace{\mathcal{E}_a + \mathcal{E}_b + C_{ab} - J_{ab}(S_1^2 + S_2^2) + J_{ab}}_{\text{const.}} - 2 J_{ab}\, S_1 \cdot S_2$$

$$\mathcal{E} = \underline{\mathcal{E}_{const}} - \underbrace{2 J_{ab}\, S_1 \cdot S_2}$$

$$H = -\text{"}J\text{"}\; S_1 \cdot S_2 \quad \text{upto const.}$$





$$H = -t \sum_{\sigma} a_{i\sigma}^{+} a_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$|\uparrow\downarrow\rangle \; |\downarrow\uparrow\rangle \; |\uparrow\downarrow\; 0\rangle \; |0\; \uparrow\downarrow\rangle \longrightarrow$ Hilbert space

$$\begin{array}{c c} \langle \uparrow \downarrow | & \\ \langle \downarrow \uparrow | & \\ \langle \uparrow\downarrow\; 0 | & \\ \langle 0\; \uparrow\downarrow | & \end{array} \left(\quad ? \quad \right)$$

$\rightarrow$ Hilbert space

$$H = +\text{"}J\text{"}\; S_i \cdot S_2$$

$$\downarrow$$

$$\langle \psi_j | H | \psi_i \rangle$$

$$1\,\text{eV} \sim 1.6 \times 10^{-19}\ \text{J}$$

$$1\,\text{meV} = 10^{-3}\ \text{eV}$$

$$1\,\text{meV} \sim 10\ \text{K}$$

$t \sim 1\,eV$
$\sim 0.5\,eV$ } $\quad U/t \sim 8$

$J_{AF} \sim \frac{4t^2}{U} \sim 0.25\ ev \sim 100\ meV$

$J \sim 3 - 10\ meV$

$\sim 0.1\ meV$ spin-orbit coupled

$-t\, a_{i\sigma}^{+} a_{j\sigma}$

Start $\quad$ "hop" $\quad$ "hop" End

$\uparrow \ \downarrow \ \longrightarrow \ \uparrow\downarrow \ \ 0 \ \longrightarrow \ \downarrow \ \uparrow$

$$S_1 \cdot S_2 = \frac{S_1^+ S_2^- + S_1^- S_2^+}{2} + S_1^z S_2^z$$

$\uparrow \ \downarrow \ \Longrightarrow \ \downarrow \ \uparrow$

$S_1^- \ S_2^+$

$\uparrow \ \uparrow$

$S_1 \cdot S_2 \qquad H = J \sum_{\langle ij \rangle} S_i \cdot S_j$

Kubo & Anderson $\sim$ 1950's spin wave theory

$S \longrightarrow$ bosons

$\uparrow \uparrow \uparrow$

$\uparrow \uparrow \uparrow$ ✓ GS ✓

$\uparrow \uparrow \uparrow$

$$S_i^+ = \sqrt{2S}\left(1 - \frac{a_i^+ a_i}{2S}\right)^{1/2} a_i \quad ✓$$

$$S_i^- = \sqrt{2S}\, a_i^+ \left(1 - \frac{a_i^+ a_i}{2S}\right)^{1/2}$$

$$(1 - x)^{1/2} \simeq 1 - \frac{1}{2}x + \cdots$$

$S \to$ large

SWT if I have ground state

$$[S_i^+, S_i^-] = 2S_i^z$$

$$[a_j, a_i^+] = \delta_{ji} \qquad [a_j, a_i] = [a_j^+, a_i^+] = 0$$

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

$$H = \frac{S_i^+ S_j^- + S_i^- S_j^+}{2} + S_i^z S_j^z$$

$$a_j = \frac{1}{\sqrt{N}} \sum_j e^{-ik \cdot r_j} b_k$$

$$a_j^{+} = \frac{1}{\sqrt{N}} \sum_j e^{+ik\cdot r_j} \, b_k^{+}$$

$\Big\} \downarrow$ math with ops

$$H \simeq -\frac{1}{2} J z S^2 + \frac{JzS}{2} \sum_k 2 b_k^{+} b_k - \underline{\gamma_k} \, \underline{b_k b_k^{+}} - \underline{\gamma_{-k}} \, b_k^{+} b_k$$

$z \Downarrow$ coordination

$S =$ spin

$z =$ coordination

$$\gamma_k = \sum_{\delta} 1 - \cos(\vec{k}\cdot\vec{\delta})$$

δ: all nearest neighbor vectors

$b_k^{+} b_k$

$[b_k, b_k^{+}] = 1$

$b_k b_k^{+} = 1 + b_k^{+} b_k$

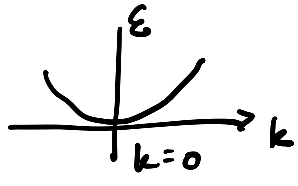
$$\gamma_k \sim J(1 - \cos(ka))$$

$k \simeq$ small

$$\cos(ka) \simeq 1 - \frac{(ka)^2}{2} + \dots$$

$$\gamma_k \sim J(ka)^2$$

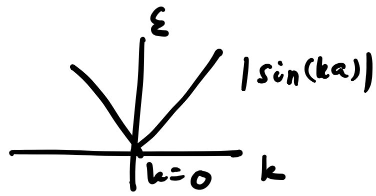
<u>FM</u>



$J(ka)^2$

$\uparrow\uparrow\uparrow\uparrow$

<u>AFM</u>



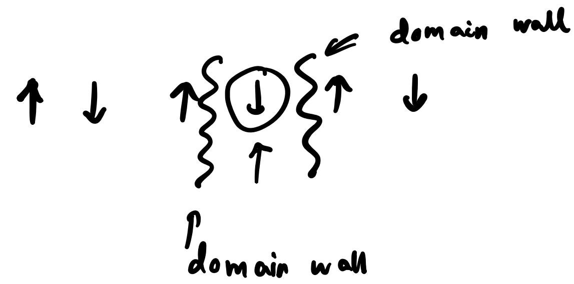
$\underline{\varepsilon \sim J|ka|}$

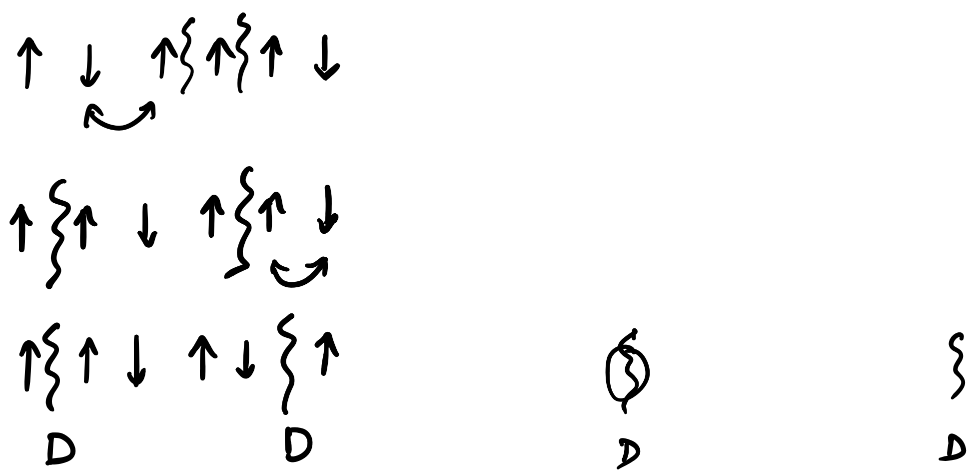
$\uparrow\downarrow \; \uparrow\downarrow \; \uparrow\downarrow$

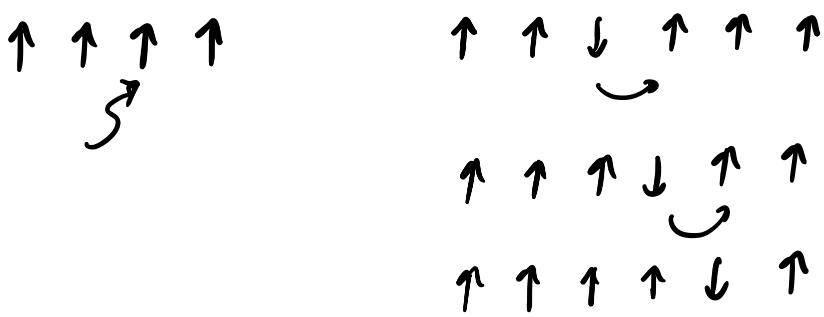
bipartite

low dimensions — observable!

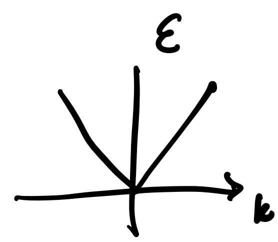
AFM order can be destroyed







"fractionalized spin"



SWT ✓