4 Interacting fermions

4.1 Q: whence spin-spin interactions?

2 Distinguishable spinless particles.

$$H = h_0(1) + h_0(2) + \underbrace{V(r_1, r_2)}_{= V(r_2, r_1)}$$

$$\begin{cases} h_0 \psi_\alpha = \epsilon_\alpha \psi_\alpha \\ h_0 \psi_\beta = \epsilon_\beta \psi_\beta \end{cases}$$

TRIAL WAVE f'ns:

$$\left[\begin{array}{l} \Psi_{S/A} \equiv \dfrac{\left(\Psi_{\alpha\beta} \pm \Psi_{\beta\alpha}\right)}{\sqrt{2}} \\[2ex] \Psi_{\alpha\beta}(r_1, r_2) \equiv \psi_\alpha(r_1)\,\psi_\beta(r_2) \end{array}\right.$$

$$E_{S/A} = \langle \Psi_{S/A} | \hat{H} | \Psi_{S/A} \rangle = \epsilon_\alpha + \epsilon_\beta + \int d^d r_1 \int d^d r_2\, \Psi^*_{S/A}(r_1, r_2)\, V(r_1, r_2)\, \Psi_{S/A}(r_1, r_2)$$

$$= \epsilon_\alpha + \epsilon_\beta + I \mp J.$$

$$E_{S/A} = \epsilon_\alpha + \epsilon_\beta + \frac{1}{2}\Big(\int_{1,2} \Psi^*_{\alpha\beta} V \Psi_{\alpha\beta} + \int_{1,2} \Psi^*_{\beta\alpha} V \Psi_{\beta\alpha}$$
$$\pm \int_{1,2} \Psi^*_{\alpha\beta} V \Psi_{\beta\alpha} \pm \int_{1,2} \Psi^*_{\beta\alpha} V \Psi_{\alpha\beta}$$
$$= \epsilon_\alpha + \epsilon_\beta + \underbrace{\int_{1,2} \Psi^*_{\alpha\beta} V \Psi_{\alpha\beta}}_{I} \pm \underbrace{\int_{1,2} \psi^*_{\beta\alpha} V \psi_{\alpha\beta}}_{-J}$$
$$= \epsilon_\alpha + \epsilon_\beta + I \mp J$$

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spinful fermions:

$$H = \underbrace{\sum_\alpha a^+_{\alpha\sigma} a_{\alpha\sigma} \epsilon_\alpha}_{h_0} + \int d^d r_1 \int d^d r_2 V(r_1, r_2) \times$$
$$\psi^+_{r_1\sigma} \psi^+_{r_2\sigma'} \psi_{r_2\sigma'} \psi_{r_1\sigma}$$

$$\left(a^+_{\alpha\sigma} = \int dr\, u_\alpha(r) \psi^+_{r\sigma} \right)$$

Note: • $[H, \vec{S}] = 0$ $\quad \vec{S} \equiv \sum_r \frac{1}{2} \psi^+_r \vec{\sigma} \psi_r$

• H is spin-independent.

all states of 2 fermions in 2 orbitals α, β.

$\boxed{\alpha \neq \beta}$ $$a^\dagger_{\alpha\sigma} a^\dagger_{\beta\sigma'} |0\rangle \overset{F}{=} - a^\dagger_{\beta\sigma'} a^\dagger_{\alpha\sigma} |0\rangle$$

totally antisymmetric (AS).

$$\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$$

σ σ'

singlet is AS under $\sigma \leftrightarrow \sigma'$

triplet is sym.

singlet, orbitally symmetric: $$|S\rangle = \frac{1}{\sqrt{2}}\left(a^\dagger_{\alpha\uparrow} a^\dagger_{\beta\downarrow} - a^\dagger_{\alpha\downarrow} a^\dagger_{\beta\uparrow}\right)|0\rangle$$
$$= \frac{1}{\sqrt{2}} \epsilon_{\sigma\sigma'} a^\dagger_{\alpha\sigma} a^\dagger_{\alpha\sigma'} |0\rangle$$
$$\left(\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma^y\right)$$

triplet orbitally AS:
$$|A,1\rangle = a^\dagger_{\alpha\uparrow} a^\dagger_{\beta\uparrow} |0\rangle$$
$$|A,0\rangle = \frac{1}{\sqrt{2}}\left(a^\dagger_{\alpha\uparrow} a^\dagger_{\beta\downarrow} + a^\dagger_{\alpha\downarrow} a^\dagger_{\beta\uparrow}\right)|0\rangle$$
$$|A,-1\rangle = a^\dagger_{\alpha\downarrow} a^\dagger_{\beta\downarrow} |0\rangle.$$

wavef'ns:

$$\langle r_1\sigma, r_2\sigma' | S\rangle = \langle 0|\psi_{r_2\sigma'}\psi_{r_1\sigma}|S\rangle$$

$$= \underbrace{\Psi_S(r_1,r_2)}_{\text{symmetric}}\underbrace{\left(\frac{\delta_{\sigma\uparrow}\delta_{\sigma'\downarrow}-\delta_{\sigma\downarrow}\delta_{\sigma'\uparrow}}{\sqrt{2}}\right)}_{\text{singlet}}$$

$$\langle r_1\sigma, r_2\sigma' | A, m^z\rangle = \Psi_A(r_1,r_2)\,\psi_{m^z}(\sigma,\sigma')$$

Note: $|S\rangle$, $|A, m^z\rangle$ are eigenstates of S^z, $\vec{S}^2$ $\quad \vec{S} = \sum_r \frac{1}{2}\psi^\dagger_{r\sigma}\vec{\sigma}_{\sigma\sigma'}\psi_{r\sigma'}$

	$\vec{S}^2 = s(s+1)$	$\frac{s(s+1)}{2}$
$s=0$ singlet	0	0
$s=1$ triplet	2	1
$s=\frac{1}{2}$	$\frac{1}{2}(\frac{1}{2}+1) = 3/4$	

$$H_{eff} = \langle S/A|H|S/A\rangle = E_{S/A}$$

$$= \epsilon_\alpha + \epsilon_\beta + I \mp J = E_S + (E_A - E_S)\cdot\frac{s(s+1)}{2}$$

$$H_{eff} = E_s + 2J\,\frac{\vec{S}\cdot\vec{S}}{2} = \underline{\underline{2J\,\vec{S}_1\cdot\vec{S}_2 + \text{const}}}$$

$$\vec{S}\cdot\vec{S} = (S_1+S_2)^2 = \underbrace{S_1^2}_{3/4} + \underbrace{S_2^2}_{3/4} + 2\vec{S}_1\cdot\vec{S}_2$$

$$\boxed{H_{eff} = 2J\,\vec{S}_1\cdot\vec{S}_2 + \text{cts}}$$

$$J = -\iint d^d r_1\, d^d r_2\, \Psi^*_{\alpha\beta}(r_1 r_2)\, V\, \Psi_{\beta\alpha}(r_1 r_2)$$

"exchange integral".

4.2 Ordering in FERMI systems

$$\vec{S}_r = \psi^+_{r\sigma}\,\tfrac{1}{2}\,\vec{\sigma}_{\sigma\sigma'}\,\psi_{r\sigma'}$$

$m = \sum_r \langle S^z_r \rangle$ → diagonal long-range order for fermions.

$^4He = 2e^- + 2p + 2n$

<u>BUT:</u> evals of ρ_1 (fermions) ≤ 1.

If $\rho = \sum_s p_s |\psi_s\rangle\langle\psi_s|$

$$\rho_2(\underbrace{r_1\sigma_1 r_2\sigma_2}_{1\ldots(2V)^2};\ \underbrace{r_1'\sigma_1' r_2'\sigma_2'}) = \sum_s p_s \sum_{\substack{\sigma_3\ldots\sigma_N \\ r_3\ldots r_N}} \Psi_s^*(r_1\sigma_1 r_2\sigma_2 \ldots r_N\sigma_N)$$

$$\Psi_s(r_1'\sigma_1' r_2'\sigma_2' \cdot r_3\sigma_3 \ldots r_N\sigma_N)$$

$V =$ # of sites

$(2V)^2 \times (2V)^2$ matrix

- $= \mathcal{J}\ \rho_2(r_2\sigma_2 r_1\sigma_1 ; r_1'\sigma_1' r_2'\sigma_2')$

- <u>useful</u>: $\langle V\rangle_\rho = \sum_{\sigma_1\sigma_2}\sum_{\sigma_1\sigma_2} V(r_1 - r_2)\rho_2(12;12)$

$$\rho_2(r_1\sigma_1 r_2\sigma_2 ; r_1\sigma_1 r_2\sigma_2) \propto g_{\sigma_1\sigma_2}(r_1 - r_2)$$

pair correlator.

- $\rho_2(r_1\sigma_1 r_2\sigma_2 ; r_1'\sigma_1' r_2'\sigma_2') = \frac{1}{N(N-1)} \langle \psi^\dagger_{r_1\sigma_1} \psi^\dagger_{r_2\sigma_2} \psi_{r_2\sigma_2} \psi_{r_1\sigma_1} \rangle$

- $\mathrm{tr}\, \rho_2 = 1$

- $\rho_2^*(r_1'\sigma_1' r_2'\sigma_2' ; r_1\sigma_1 r_2\sigma_2) = \rho(r_1\sigma_1 r_2\sigma_2 ; r_1'\sigma_1' r_2'\sigma_2')$

ie $\rho_2 = \rho_2^\dagger$ as a $(2V)^2 \times (2V)^2$ matrix

- $\rho_2 \geq 0 \Rightarrow$ evals are ≥ 0.

$$\rho_2(r_1\sigma_1 r_2\sigma_2 ; r_1'\sigma_1' r_2'\sigma_2') = \sum_i \underbrace{\frac{n_i}{N(N-1)}}_{\text{evals}} \underbrace{\chi_i^*(r_1\sigma_1 r_2\sigma_2)\, \chi_i(r_1'\sigma_1' r_2'\sigma_2')}_{\text{evecs}}$$

evecs are 2-particle fermi wavef'ns. ON.

$\mathrm{tr}\,\rho_2 = 1$

$\Rightarrow \sum_i n_i = N(N-1)$.

$\Rightarrow \underline{n_1 \leq N(N-1)}$.

$\chi_i(r_1\sigma_1 r_2\sigma_2) = -\chi_i(r_2\sigma_2 r_1\sigma_1)$

w/ N particles and s orbitals

$$n_i \leq \frac{N(s-N+2)}{s} \xrightarrow{s>>N} N$$

let $f \equiv \frac{N}{s}$ fixed as $N\to\infty$

"filling fraction"

$s = N/f$

$$\Rightarrow n_i \overset{N\to\infty}{\leq} \frac{N(\frac{N}{f}-N)}{N/f}$$

$$= N \frac{\frac{1}{f}-1}{1/f}\frac{f}{f}$$

$$= N(1-f).$$

$$\boxed{n_i \leq O(N)}$$

Df: If all $n_i \sim O(1)$ "normal"

If ANY $n_i \sim O(N)$ "Cooper pairing"

"pseudo-BEC".

eg free fermions: $\hat{n}_k \equiv \hat{\psi}_k^+ \hat{\psi}_k$

g.s. of $\hat{n}_k |\Psi_0\rangle = n_k |\Psi_0\rangle$

$$n_k = \begin{cases} 0 & |k| > k_F \\ 1 & |k| < k_F \end{cases}$$

$\rightarrow$ evals of ρ_2 are also 0, 1.

$\rightarrow$ interactions are required for Cooper pairing.

4.2 Instabilities of a Fermi surface to repulsive interactions

$$H = -t \sum_{\langle xy \rangle \sigma} c^{\dagger}_{x\sigma} c_{y\sigma} + h.c$$

$$+ U \sum_x (\hat{n}_x - 1)^2 \equiv H_t + H_U$$

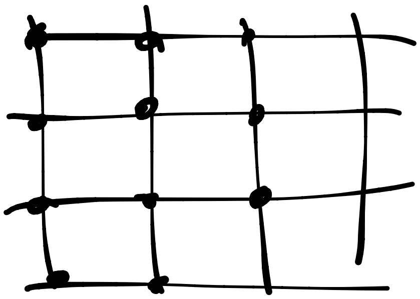
$$\hat{c}_{x\sigma} \equiv \hat{\psi}_{x,\sigma} \equiv \hat{a}_{x\sigma}$$

$$\hat{n}_x \equiv c^\dagger_{x\uparrow} c_{x\uparrow} + c^\dagger_{x\downarrow} c_{x\downarrow} = \sum_\sigma c^\dagger_{x\sigma} c_{x\sigma}.$$

Assume transl. inv:

$$\boxed{U = 0}$$

$$H_t = \sum_k \underset{\sim}{\epsilon_k}\, c^\dagger_{k\sigma} c_{k\sigma}$$



$\rightarrow a \leftarrow$

$$\longrightarrow \epsilon_k = -2t(\cos k_x a + \cos k_y a)$$

$$[H, \hat{N}] = 0$$

$$\hat{N} \equiv \sum_x \hat{n}_x .$$

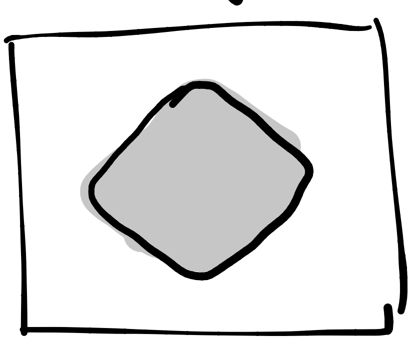
filling fraction

$$f = \frac{\#\text{ of particles}}{\text{single-particle state}} = \frac{N}{2V}$$

spin.

$$\boxed{\text{Metal}}$$

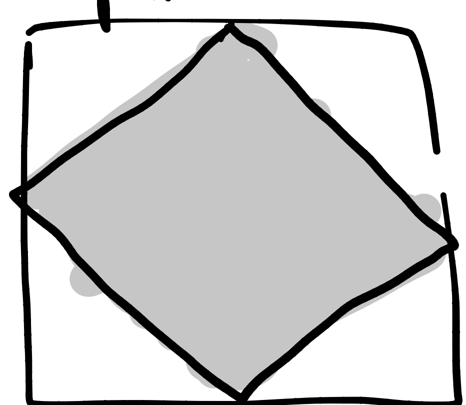
$V \equiv \#$ of sites.



k_y

k_x

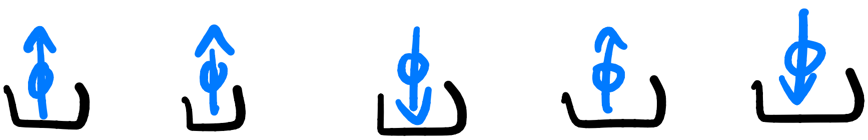
$f < \frac{1}{2}$



$f = \frac{1}{2}$

$\boxed{U=\infty}$ $\quad \underline{f=\frac{1}{2}}$. $\quad H_U = U\sum_x (n_x-1)^2$

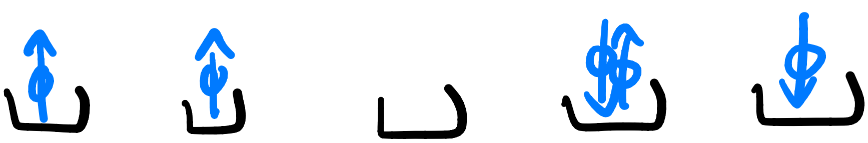
wants one particle per site.

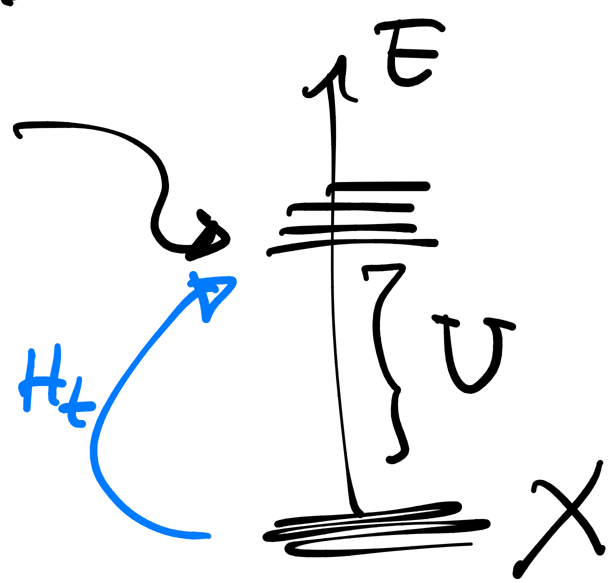


degenerate ground space of dim $= 2^V = 2^N$

$X \simeq \bigotimes_x \mathcal{H}_{1/2}$

This is a Mott Insulator.





$E - E_0 \sim U$

Degen. Pert Thy w/

$\boxed{\frac{U}{t} \gg 1}$

$\Delta H = H_t$

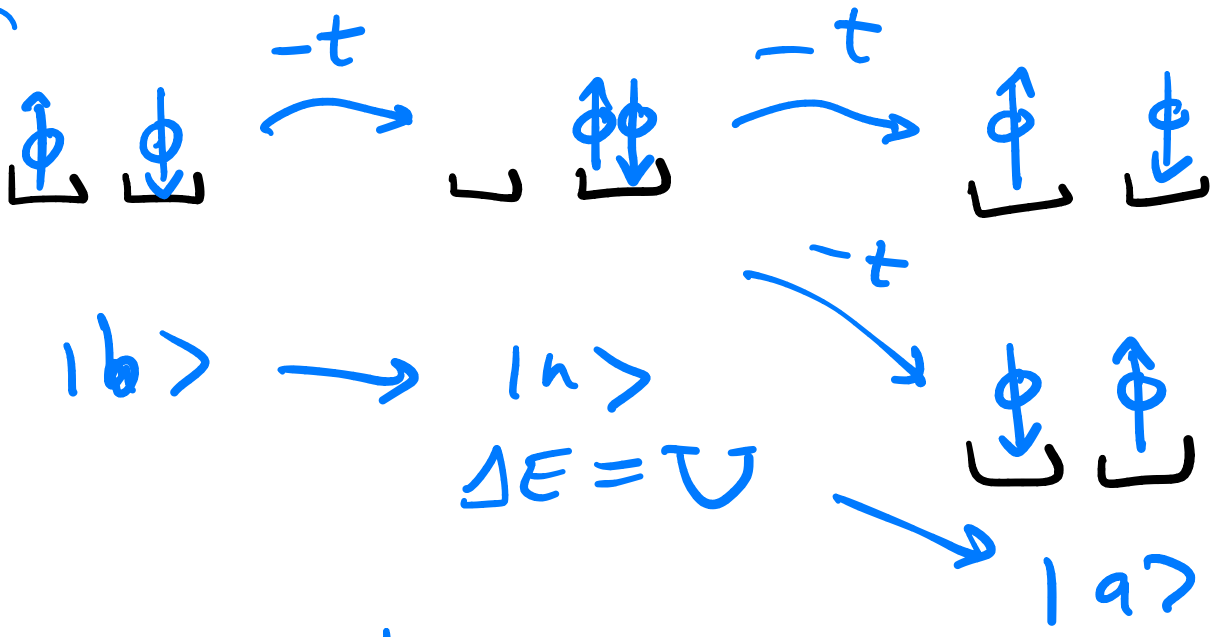
1st order term:

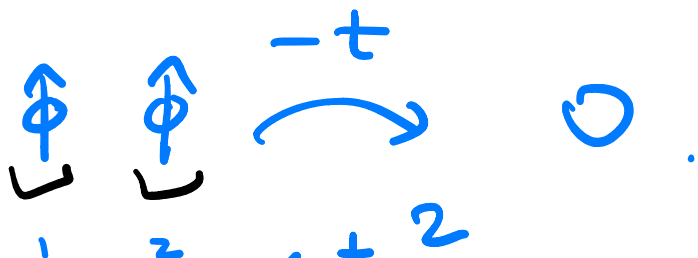
$\langle a|H_t|b\rangle = 0$

for $|a\rangle, |b\rangle \in X$.

2d order:

$$\langle a|H_{eff}|b\rangle = -\sum_{n\notin X}\frac{\langle a|\Delta H|n\rangle\langle n|\Delta H|b\rangle}{E_n - E_X} \qquad E_n - E_X \equiv \Delta E$$





$$(a^{+}_{2\uparrow})^2 = 0.$$

$$\vec{S} = \sum_r c^{+}_{r\sigma}\sigma_{\sigma\sigma'}c_{r\sigma'}$$

$$[H, \vec{S}] = 0.$$

a

$$|1\rangle = a^{+}_{1\uparrow}a^{+}_{2\uparrow}|0\rangle$$

$$= -a^{+}_{2\uparrow}a^{+}_{1\uparrow}|0\rangle$$

$$|2\rangle = \ldots$$

$|3\rangle$

$|4\rangle$

$n\notin X$:

$$|5\rangle = a^{+}_{1\uparrow}a^{+}_{1\downarrow}|0\rangle$$

$$|6\rangle = a^{+}_{2\uparrow}a^{+}_{2\downarrow}|0\rangle$$

$$H_{\text{eff}} = +\frac{4t^2}{U}\sum_{\langle xy\rangle} \vec{S}_x\cdot\vec{S}_y$$

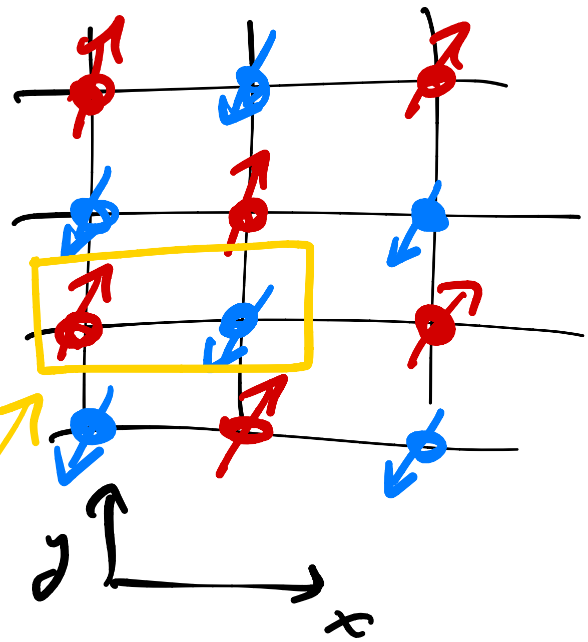
ANTIFERROMAGNET! w/ $J = \frac{4t^2}{U}$.

("superexchange")

on a bipartite lattice

$$\langle \vec{S}_{\vec{x}=(x,y)}\rangle = (-1)^{x+y}\,\hat{z}\,m$$

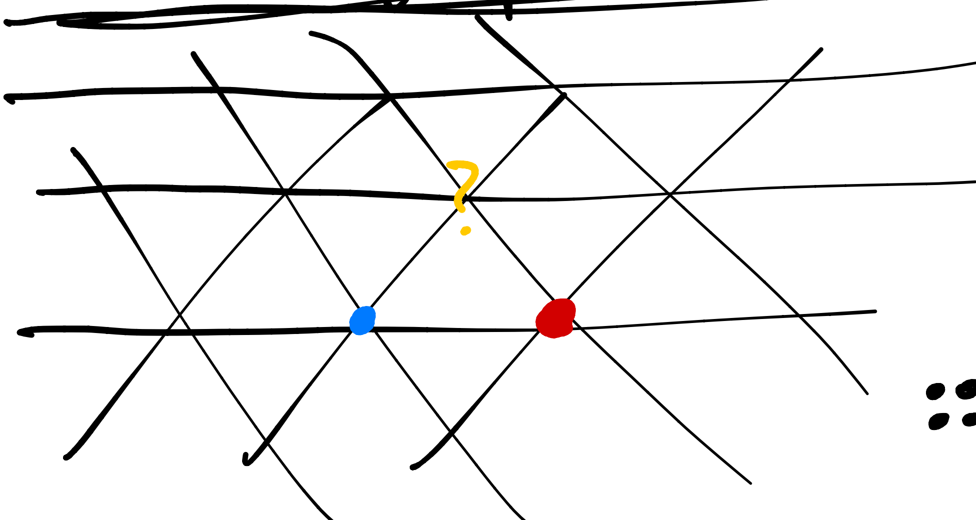
unit cell



breaks SU(2) × (translations)

→ subgroup.

"Neel state"



"FRUSTRATION"

solid : liquid

:: magnet : "spin liquid"