Part 3

the origin of magnetism and the Hubbard model.

approaches from "constructive condensed matter physics"

— o —

Why do we have spin-spin interactions $\hat{S}_x \cdot \hat{S}_y$?

the origin of magnetism.

Heisenberg 1928

fermions

- quantum many body effect of electrons
- Coulomb interaction between the electrons

naive perturbation

"exchange interaction"

connecting different levels of descriptions

electron sys. → spin sys.

Q: Do we really get macroscopic ferromagnetism in interacting many-electron systems ??

⟨Hubbard model⟩

§ Operators and states

tigh-binding description of electrons in a solid.

<u>lattice</u> $\Lambda \ni x, y, \ldots$ sites

electrons { mostly live on a site = atom
{ "hops" from a site to another

<u>creation and annihilation operators</u>

$$x \in \Lambda, \quad \sigma = \uparrow, \downarrow$$

$\hat{c}^\dagger_{x,\sigma}$ creates an electron at x with spin σ

$\hat{c}_{x,\sigma}$ annihilates

canonical anticommutation relations — in particular $(\hat{c}^\dagger_{x\sigma})^2 = 0$ Pauli priciple.

$$\{\hat{c}_{x,\sigma}, \hat{c}_{y,\tau}\} = \{\hat{c}^\dagger_{x,\sigma}, \hat{c}^\dagger_{y,\tau}\} = 0$$

$$\{\hat{c}^\dagger_{x,\sigma}, \hat{c}_{y,\tau}\} = \delta_{x,y}\,\delta_{\sigma,\tau} \quad \text{for } {}^\forall x, y, \sigma, \tau$$

$$\{\hat{A}, \hat{B}\} := \hat{A}\hat{B} + \hat{B}\hat{A}$$

<u>number operator</u>

$$\hat{n}_{x,\sigma} = \hat{c}^\dagger_{x,\sigma}\hat{c}_{x,\sigma}, \quad (\hat{n}_{x,\sigma})^2 = \hat{n}_{x,\sigma}$$

$$\hat{n}_x = \hat{n}_{x\uparrow} + \hat{n}_{x\downarrow}, \quad \hat{N} = \sum_{x \in \Lambda} \hat{n}_x$$

DATE

Spin operators

$$\hat{S}_x^{(3)} = \frac{1}{2}(\hat{n}_{x\uparrow} - \hat{n}_{x\downarrow})$$

$$\hat{S}_x^{+} = \hat{c}_{x\uparrow}^{\dagger}\hat{c}_{x\downarrow}, \quad \hat{S}_x^{-} = \hat{c}_{x\downarrow}^{\dagger}\hat{c}_{x\uparrow}$$

$$\hat{\mathbf{S}}_x = (\hat{S}_x^{(1)}, \hat{S}_x^{(2)}, \hat{S}_x^{(3)})$$

spin operators

→ See the problem.

Total spin op. $\hat{\mathbf{S}}_{tot} = \sum_{x\in\Lambda} \hat{\mathbf{S}}_x$

the e.v. of $(\hat{\mathbf{S}}_{tot})^2 \rightarrow S_{tot}(S_{tot}+1)$

Hilbert space

Φ_{vac} unique state with no electrons

$$\|\Phi_{vac}\| = 1, \quad \hat{c}_{x,\sigma}\Phi_{vac} = 0 \text{ for } {}^\forall x, \sigma.$$

$\mathcal{H}_N$: Hilbert space with N electrons
$(0 \leq N \leq 2|\Lambda|)$

basis states

$$\mathcal{U} \subset \Lambda, \ \mathcal{D} \subset \Lambda \quad \text{with } |\mathcal{U}| + |\mathcal{D}| = N$$

$$\Psi_{\mathcal{U},\mathcal{D}} := \left(\prod_{x\in\mathcal{U}} c^\dagger_{x\uparrow}\right)\left(\prod_{x\in\mathcal{D}} c^\dagger_{x\downarrow}\right)\Phi_{vac}$$

$$\cancel{\hat{N}\,\Psi_{\mathcal{U},\mathcal{D}} = N\,\Psi_{\mathcal{U},\mathcal{D}}}$$

in $\mathcal{H}_N$, the possible values of S_{tot} are

$$0, 1, 2, \cdots, \frac{N}{2}$$

or

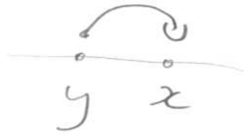
$$\frac{1}{2}, \frac{3}{2}, \cdots, \frac{N}{2}$$

§ Hopping Hamiltonian

hopping amplitude $t_{xy} = t_{yx} \in \mathbb{R}$

(t_{xx} on-site potential)

$$\hat{H}_{\mathrm{hop}} = \sum_{\substack{x,y\in\Lambda \\ \sigma=\uparrow,\downarrow}} t_{xy}\, \hat{c}^{\dagger}_{x\sigma} \hat{c}_{y\sigma}$$



$$[\hat{S}^{(\alpha)}_{\mathrm{tot}}, \hat{H}_{\mathrm{hop}}] = 0, \quad [\hat{N}, \hat{H}_{\mathrm{hop}}] = 0$$

<u>Single-electron energy eigenstates</u>

tight-binding Sch. eq.

$$\sum_{y} t_{xy} \psi^{(j)}_{y} = \epsilon_j \psi^{(j)}_{x} \quad \text{for } \forall x \in \Lambda$$

$$(\psi^{(j)}_x \in \mathbb{C}) \qquad (j = 1, 2, \cdots, |\Lambda|)$$

$$\sum_{x} (\psi^{(j)}_x)^* \psi^{(j')}_x = \delta_{j,j'}, \qquad \sum_{j} \psi^{(j)}_x (\psi^{(j)}_y)^* = \delta_{xy}$$

(orthonormal) (complete)

$\psi^{(j)}_x$ is usually represents a "wave"

corresponding operator

$$\hat{d}^{\dagger}_{j,\sigma} := \sum_{x\in\Lambda} \psi^{(j)}_x c^{\dagger}_{x\sigma}, \quad \hat{n}_{j\sigma} = \hat{d}^{\dagger}_{j\sigma} \hat{d}_{j\sigma}$$

$$\{\hat{d}^{\dagger}_{j,\sigma}, \hat{d}_{j',\tau}\} = \delta_{jj'} \delta_{\tau\tau'}$$

$\hat{H}_{hop}$ is ~~easily~~ diagonalized as

$$\hat{H}_{hop} = \sum_{j=1}^{|\Lambda|} \sum_{\sigma=\uparrow,\downarrow} \epsilon_j \hat{n}_{j,\sigma}$$

→ note $[\hat{n}_{j\sigma}, \hat{n}_{j'\tau}] = 0$

$$\because \sum_j \epsilon_j \hat{d}^\dagger_{j\sigma} \hat{d}_{j\sigma} = \sum_{j,x,y} \epsilon_j \psi_x^{(j)} (\psi_y^{(j)})^* \hat{c}^\dagger_{x\sigma} \hat{c}_{y\sigma}$$

$$= \sum_{j,x,y,z} t_{xz} \underbrace{\psi_z^{(j)} (\psi_y^{(j)})^*} \hat{c}^\dagger_{x\sigma} \hat{c}_{y\sigma}$$

$$= \sum_{x,y} t_{xy} \hat{c}^\dagger_{x\sigma} \hat{c}_{y\sigma}$$

eigenstates of $\hat{H}_{hop}$

$I, J \subset \{1, 2, \cdots, |\Lambda|\}$, $|I| + |J| = N$

$$\Phi_{I,J} := \underbrace{\left(\prod_{j\in I} \hat{d}^\dagger_{j\uparrow}\right)\left(\prod_{j\in J} \hat{d}^\dagger_{j\downarrow}\right) \Phi_{vac.}}$$

→ Slater determinant

then $$\hat{H}_{hop} \Phi_{I,J} = \left(\sum_{j\in I} \epsilon_j + \sum_{j\in J} \epsilon_j\right) \Phi_{I,J}$$

electrons behave as "wave"

the g.s. of $\hat{H}_{hop}$

if N even, $\epsilon_j < \epsilon_{j+1}$ $(j = 1, 2, \dots, |\Lambda| - 1)$

then the g.s is unique

$$\Phi_{GS} = \left(\prod_{j=1}^{N/2} d^\dagger_{j\uparrow} d^\dagger_{j\downarrow} \right) \Phi_{vac}$$

uniqueness implies

$$\hat{S}^{(\alpha)}_{tot} \, \Phi_{GS} = 0 \qquad (S_{tot} = 0)$$

Pauli paramagnetism

Hub-1

(a) Show that $\hat{\mathbf{S}}_x$ are angular momentum operators, and express $(\hat{\mathbf{S}}_x)^2$ in terms of $\hat{n}_x$

Hub-2

(a) By using the definitions and anticommutation relations, show that $\left[\hat{S}^{(\alpha)}_{tot}, \left(\sum_x \gamma_x c^\dagger_{x\uparrow} \right) \left(\sum_x \gamma_x c^\dagger_{x\downarrow} \right) \right] = 0$

for $\forall \gamma_x \in \mathbb{C}$

Show ~~Note~~ that this implies

two electrons in a single state form spin-singlet

§ interaction Hamiltonian

$$\hat{H}_{int} := U \sum_{x\in\Lambda} \hat{n}_{x\uparrow}\hat{n}_{x\downarrow} \quad , \quad U>0$$

on-site Coulomb interaction.

$$[\hat{H}_{int}, \hat{S}^{(\alpha)}_{tot}] = 0, \quad [\hat{H}_{int}, \hat{N}] = 0$$

Clearly $\hat{H}_{int} \geqq 0$

$$\hat{H}_{int}\, \Phi_{\mathcal{U},D} = U\, |\mathcal{U}\cap D|\, \Phi_{\mathcal{U},D}$$

<u>the g.s. of $\hat{H}_{int}$</u>

simply minimize $|\mathcal{U}\cap D|$

if $N \leqq |\Lambda|$

For any $\mathcal{U}, D$ s.t. $\mathcal{U}\cap D = \phi$

$$\hat{H}_{int}\, \Phi_{\mathcal{U},D} = 0 \,, \Rightarrow \Phi_{\mathcal{U}D} \text{ is a g.s.}$$

↑ ↓ ↑

○ ↑ ○

↓ ↑ ↓

g.s. are highly degenerate

$\hookrightarrow$ paramagnetism (as in the Ising at $T=\infty$)

electrons behave as "particles"

§ Hubbard model

$$\boxed{\hat{H} = \underset{\substack{\nearrow \\ \text{"wave"}}}{\hat{H}_{hop}} + \underset{\substack{\nearrow \\ \text{"particle" dualism}}}{\hat{H}_{int}}}$$

neither $\hat{H}_{hop}$ nor $\hat{H}_{int}$ favors any magnetic order

unlike the spin Hamiltonian, $\hat{H}$ itself does not suggest any favored states

BUT

"competition" between $\hat{H}_{hop}$ and $\hat{H}_{int}$

$$\Downarrow$$

nontrivial order (such as ferromagnetism)

⟨Half-filled system⟩

$0 \leq N \leq 2|\Lambda|$

the case $N = |\Lambda|$ half-filled

§ Limitting cases

$U=0$

$$\Phi_{GS} = \left(\prod_{j=1}^{N/2} \hat{d}^\dagger_{j\uparrow} \hat{d}^\dagger_{j\downarrow} \right) \Phi_{vac}$$

unique g.s. (if $\epsilon_{\frac{N}{2}} < \epsilon_{\frac{N}{2}+1}$)

$S_{tot} = 0$

metallic if t_{xy} describes a single band.

$U = \infty$

$\Phi_{GS} = \Phi_{\mathcal{U},D}$ with $\forall \mathcal{U}, D$ s.t. $\mathcal{U} \cup D = \Lambda$.

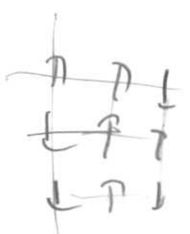
we can also write

$$\Phi_{GS} = \Phi^{\sigma} = \left(\prod_{x\in\Lambda} c^\dagger_{x,\sigma_x} \right) \Phi_{vac}.$$

with $\forall \sigma = (\sigma_x)_{x\in\Lambda}$, $\sigma_x = \uparrow, \downarrow$

spin configuration $\longleftrightarrow$ g.s.

highly degenerate g.s.



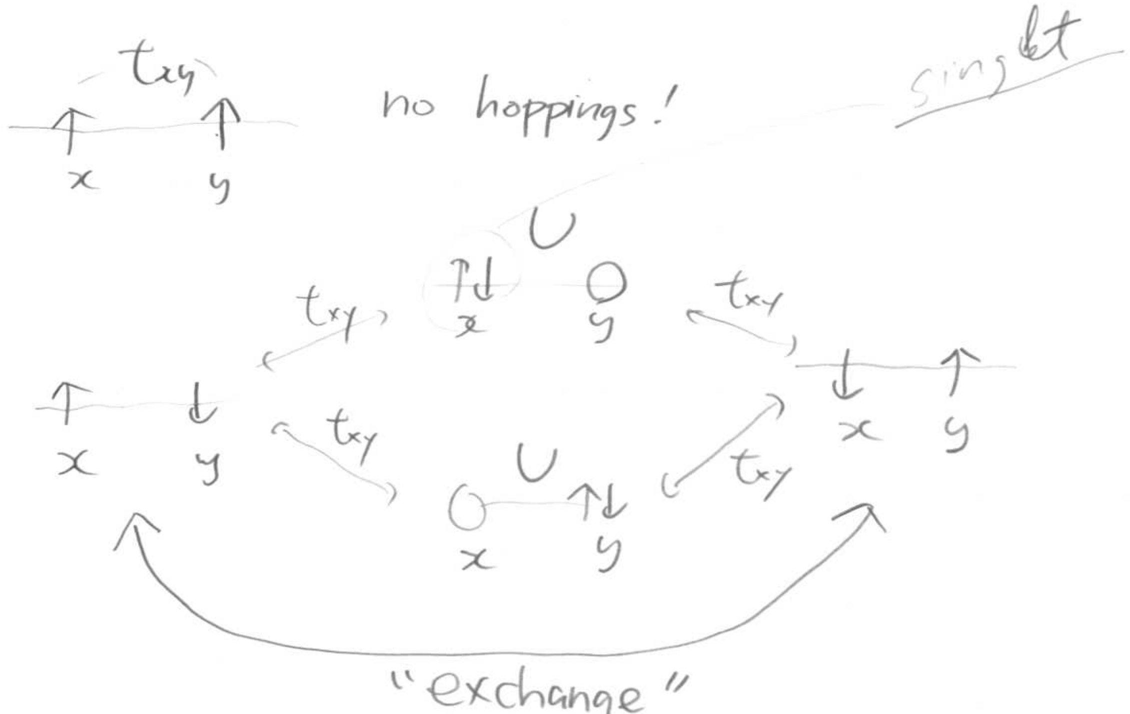
no electrons can hop

Mott insulator

§ Perturbation

$|t_{xy}| \ll U \rightarrow$ perturbation from the highly-degenerate g.s. Ψ^{Φ}.

2nd order pert. in t_{xy}



the energy of the spin singlet is lowered.

effective Hamiltonian.

$$\hat{H}_{eff} \simeq \sum_{x,y \in \Lambda} \frac{2(t_{xy})^2}{U} \left(\hat{\mathbb{S}}_x \cdot \hat{\mathbb{S}}_y - \frac{1}{4} \right)$$

Heisenberg AF

<u>Conjecture</u> Low energy properties of the Hubbard model with $N = |\Lambda|$ and $|t_{xy}| \ll U$ are described by the Heisenberg AF.

§ Lieb's thorem

<u>Theorem</u>(Lieb 1989) $|\Lambda|$ even, $\Lambda = A \cup B$ (with $A \cap B = \phi$),
$t_{xy} \neq 0$ only when $x \in A, y \in B$ or $x \in B, y \in A$.
Λ is connected via nonvanishing t_{xy}.
Then for any $U > 0$, the g.s. of the Hubbard model with $N = |\Lambda|$ have $S_{tot} = \frac{1}{2} \big| |A| - |B| \big|$, and are nondegenerate apart from the trivial spin degeneracy.

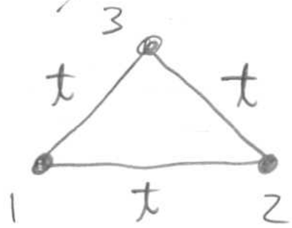
BUT THIS is FOR $t > 0$

the same as the g.s. of the Heisenberg AF, but the proof is much harder.

No rigorous resuts on AF order.

⟨Toy model for Ferromagnetism⟩

We need to move away from the half-filling to get ferromagnetism



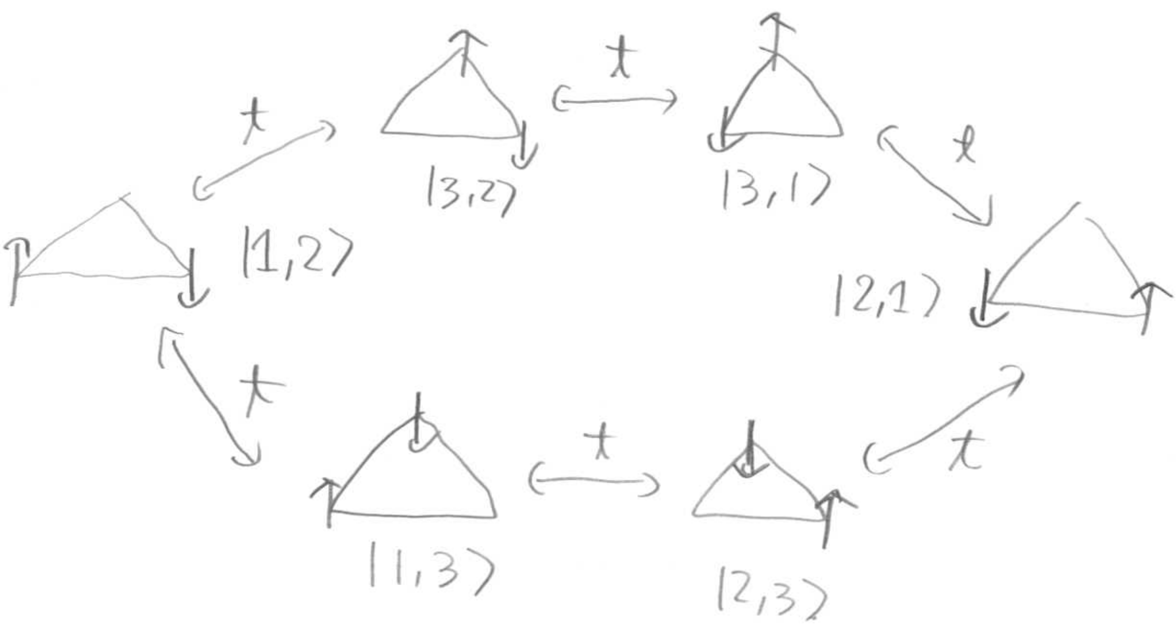
$N=2$

$U=\infty \rightarrow$ no double occupancies

basis states $|x,y\rangle = C^\dagger_{x\uparrow} C^\dagger_{y\downarrow} \Phi_{vac}$

$(x,y) = (1,2), (1,3), (2,3), (2,1), (3,1), (2,3)$

matrix elements of $\hat{H}$



the ground state

$t<0 \quad \Phi_{GS}^{(1)} = |1,2\rangle + |3,2\rangle + |3,1\rangle + |2,1\rangle + |2,3\rangle + |1,3\rangle$

$t>0 \quad \Phi_{GS}^{(2)} = |1,2\rangle - |3,2\rangle + |3,1\rangle - |2,1\rangle + |2,3\rangle - |1,3\rangle$

$$|1,2\rangle + |2,1\rangle = (c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{2\uparrow}c^\dagger_{1\downarrow})\Phi_{vac}$$
$$= \underbrace{(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} - c^\dagger_{1\downarrow}c^\dagger_{2\uparrow})\Phi_{vac}}$$

spin-singlet. $S_{tot}=0$

$$|1,2\rangle - |2,1\rangle = (c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{1\downarrow}c^\dagger_{2\uparrow})\Phi_{vac}$$

triplet $S_{tot}=1$

the g.s. exhibits "ferromagnetism" if $t>0$

delicate phenomenon which depends on the sign of t_{xy}

More generally, t_{11}, t_{22}, t_{33} arbitrary $t_{12}=t_{21}$, $t_{13}=t_{31}$, $t_{23}=t_{32}$.

the g.s. has $\begin{cases} S_{tot}=0 & \text{if } t_{12}t_{23}t_{31}<0 \\ S_{tot}=1 & \text{if } t_{12}t_{23}t_{31}>0 \end{cases}$

Hub-~~A~~3 Prove this. (Use Perron-Frobenius)

Hub-~~B~~4 Examine the cases with $t_{xy}\in\mathbb{C}$, $(t_{xy})^*=t_{yx}$

ferro g.s. in bulk?

< Flat-band ferromagnetism >

1st rigorous example

Nagaoka-Thouless 65 — $U=\infty$, $N=|\Lambda|-1$ — single hole!

↕ more than 25 years!

flat-band ferro Mielke 91, Tasaki 92. — $D=\infty$ ← (density of state)

Stoner criterion ← extremely heuristic

UD large

↓

ferro

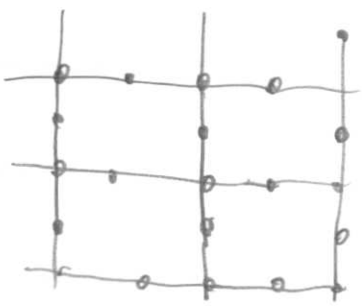
§ Model and the theorem

$\mathcal{M}$: $L\times\cdots\times L$ d-dim. hypercubic lattice (p.b.c)

$\Downarrow$
$x, y, \ldots$

$\mathcal{O}$: the set of sites at the center of bonds of $\mathcal{M}$

$\Downarrow$
$u, v, \ldots$



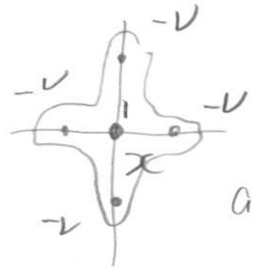
$\Lambda = \mathcal{M} \cup \mathcal{O}$

↑ decorated hyper cubic lattice

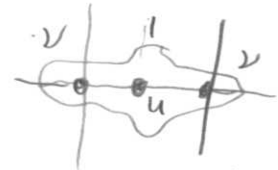
fix $\nu > 0$

fermion operators

$$\begin{cases} x \in \mathcal{M} & \hat{a}_{x\sigma} = \hat{c}_{x\sigma} - \nu \displaystyle\sum_{\substack{u\in\mathcal{O} \\ (|x-u|=1/2)}} \hat{c}_{u,\sigma} \\ u \in \mathcal{O} & \hat{b}_{u\sigma} = \hat{c}_{u\sigma} + \nu \displaystyle\sum_{\substack{x\in\mathcal{M} \\ (|x-u|=1/2)}} \hat{c}_{x\sigma} \end{cases}$$



a-state



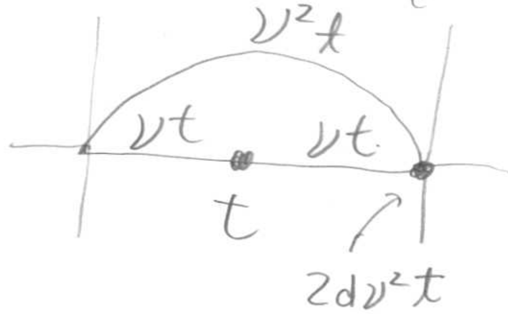
b-state

then $t > 0$

we let

$$\hat{H}_{hop} = t \sum_{\substack{u \in \mathcal{O} \\ \sigma = \uparrow,\downarrow}} \hat{b}^\dagger_{u,\sigma} \hat{b}_{u,\sigma} = \sum_{\substack{x,y \\ \sigma}} t_{xy} c^\dagger_{x\sigma} c_{y\sigma}$$

$$\hat{H}_{int} = U \sum_{z \in \Lambda} \hat{n}_{z\uparrow} \hat{n}_{z\downarrow}$$



looks like the toy model!

nearest + next nearest hoppings (which are "fine-tuned")

<u>Theorem</u> (Tasaki 92) Let $N = |\mathcal{M}| (= L^d)$

For $\forall\, U > 0$, the g.s. have $S_{tot} = N/2$ and are nondegenerate apart from the trivial $(2S_{tot}+1)$-fold degeneracy.

$\downarrow$

saturated ferromagnetism at zero temp.

§ flat-band

- $\{\hat{a}^\dagger_{x\sigma}, \hat{b}_{u\tau}\} = 0$ for $\forall x, u, \sigma, \tau$
- $|\mathcal{M}|$ states $\hat{a}^\dagger_{x\sigma}\Phi_{vac}$ with $x \in \mathcal{M}$ are independent

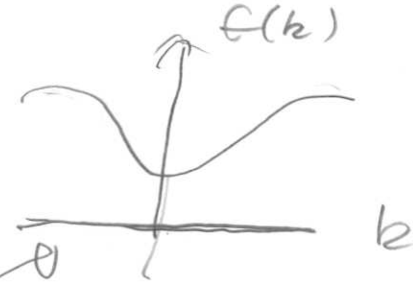
$$[\hat{H}_{hop}, \hat{a}^\dagger_{x\sigma}] = 0$$

$$\therefore \quad \hat{H}_{hop}\hat{a}^\dagger_{x\sigma}\Phi_{vac} = \hat{a}^\dagger_{x\sigma}\underbrace{\hat{H}_{hop}\Phi_{vac}}_{=0} = 0$$

Since $\hat{H}_{hop} \geq 0$, $\hat{a}^\dagger_{x\sigma}\Phi_{vac}$ is a g.s. with $N=1$

The single-electron g.s. are $\underbrace{|\mathcal{M}|}_{=L^d}$-fold degenerate!

single-electron energy spectrum (solution of the single-electron Sch. eq. for our t_{xy})



flat-band

the result of artificial "fine-tuning"

§ Proof of the theorem

$\hat{H}_{hop} \geq 0, \ \hat{H}_{int} \geq 0 \Rightarrow \hat{H} \geq 0 \quad \therefore E_{GS} \geq 0$

useful facts

$\hat{A} \geq 0, \hat{B} \geq 0$
$(\hat{A}+\hat{B})\Phi = 0$
$\Downarrow$
$\hat{A}\Phi = 0$ and $\hat{B}\Phi = 0$

$b^\dagger b \Phi = 0$
$\Downarrow$
$b\Phi = 0$

1) a g.s.

Let $\Phi_\uparrow = \left(\prod_{x \in \Lambda_1} a^\dagger_{x\uparrow}\right) \Phi_{vac}$

$$\begin{cases} \hat{H}_{hop} \Phi_\uparrow = \left(\prod_x a^\dagger_{x\uparrow}\right) \hat{H}_{hop} \Phi_{vac} = 0 \\ \hat{H}_{int} \Phi_\uparrow = 0 \end{cases}$$

$\therefore \hat{H} \Phi_\uparrow = 0 \Rightarrow \Phi_\uparrow$ is a g.s., and $E_{GS} = 0$

other g.s.?

2) general g.s.

Φ be a g.s. $\hat{H}\Phi = 0 \Rightarrow \hat{H}_{hop}\Phi = 0, \ \hat{H}_{int}\Phi = 0$

$\hat{H}_{hop} = t \sum_{u,\sigma} \hat{b}^\dagger_{u\sigma} \hat{b}_{u\sigma} \rightarrow \hat{b}_{u\sigma} \Phi = 0$ for $\forall u, \sigma$ ①

$\hat{H}_{int} = U \sum_z \hat{n}_{z\uparrow} \hat{n}_{z\downarrow} = U \sum_z (\hat{c}_{z\downarrow} \hat{c}_{z\uparrow})^\dagger \hat{c}_{z\downarrow} \hat{c}_{z\uparrow}$

$\rightarrow \hat{c}_{z\downarrow} \hat{c}_{z\uparrow} \Phi = 0$ for $\forall z$ ②

①, ② detailed conditions

You can show that

$\boxed{\text{any state can be written in terms of } a, b}$

any $= \sum (\ ) a^{\dagger} \cdots a^{\dagger} b^{\dagger} \cdots b^{\dagger} \Phi_{vac}$

• spin system representation

$\boxed{a, b \text{ complete}}$

① ⇒ no $b^{\dagger}$ states in Φ.

So any Φ is expanded as

coefficient

$$\Phi = \sum_{\substack{\mathcal{U}, \mathcal{D} \subset \Lambda \\ (|\mathcal{U}| + |\mathcal{D}| = |\Lambda|)}} \alpha_{\mathcal{U},\mathcal{D}} \left(\prod_{x \in \mathcal{U}} \hat{a}^{\dagger}_{x\uparrow} \right) \left(\prod_{x \in \mathcal{D}} \hat{a}^{\dagger}_{x\downarrow} \right) \Phi_{vac}$$

note that for $x \in \Lambda$

$$\hat{c}_{x\downarrow} \hat{c}_{x\uparrow} \hat{a}^{\dagger}_{x\uparrow} \hat{a}^{\dagger}_{x\downarrow} (\cdots\cdots) \Phi_{vac} = (\cdots) \Phi_{vac}.$$

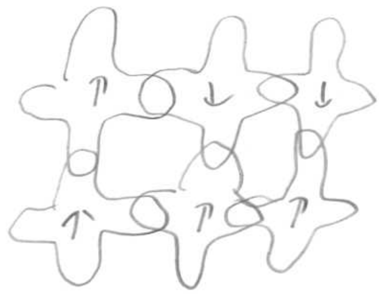
$\uparrow$ $\hat{a}$'s other than x

$$\hat{c}_{x\downarrow} \hat{c}_{x\uparrow} \underbrace{(\hat{a}^{\dagger} \cdots\cdots \hat{a}^{\dagger})}_{\text{no double } x} \Phi_{vac} = 0$$

② ⇒ $\alpha_{\mathcal{U},\mathcal{D}} \neq 0$ only when $\mathcal{U} \cap \mathcal{D} = \phi$.

$\boxed{\text{repulsion in real space} \longrightarrow \text{repulsion in state space}}$

$$\mathcal{U}\cap D=\phi \Rightarrow \mathcal{U}\cup D=\mathcal{M}$$



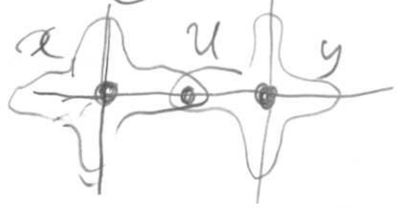
So we get the spin-system rep.

$$\Phi = \sum_{\sigma} \underbrace{\gamma_{\sigma}}_{\text{unknown const.}} \Big(\prod_{x\in\mathcal{M}} \hat{a}^\dagger_{x\sigma_x}\Big)\Phi_{vac}$$

fixed ordering

$$\sigma = (\sigma_x)_{x\in\mathcal{M}}\ ,\quad \sigma_x = \uparrow,\downarrow$$

• exchange interaction $\longleftarrow$ $\hat{c}_{u\downarrow}\hat{c}_{u\uparrow}\Phi = 0$ ② $(u\in\mathcal{O})$



$$\hat{c}_{u\downarrow}\hat{c}_{u\uparrow}\hat{a}^\dagger_{x\sigma}\hat{a}^\dagger_{y\sigma'}\overbrace{\hat{a}^\dagger\cdots\hat{a}^\dagger}^{\text{other than } x,y}\Phi_{vac}$$

$$= \begin{cases} \nu^2\, \overbrace{\hat{a}^\dagger\cdots\hat{a}^\dagger}\,\Phi_{vac} & \sigma=\uparrow,\ \sigma'=\downarrow \\ -\nu^2\, \hat{a}^\dagger\cdots\hat{a}^\dagger\,\Phi_{vac} & \sigma=\downarrow,\ \sigma'=\uparrow \\ 0 & \left\{\begin{array}{l}\sigma=\uparrow,\ \sigma'=\uparrow \\ \sigma=\downarrow\ \sigma'=\downarrow\end{array}\right. \end{cases}$$

So

$$\hat{c}_{u\downarrow}\hat{c}_{u\uparrow}\Phi = \hat{c}_{u\downarrow}\hat{c}_{u\uparrow}\sum_{\tau}\Big(\gamma_{(\uparrow,\downarrow,\tau)}\hat{a}^\dagger_{x\uparrow}\hat{a}^\dagger_{y\downarrow} + \gamma_{(\downarrow,\uparrow,\tau)}\hat{a}^\dagger_{x\downarrow}\hat{a}^\dagger_{y\uparrow}\Big)\Big(\prod_{z\in\mathcal{M}\setminus\{x,y\}}\hat{a}^\dagger_{z,\tau_z}\Big)\Phi_{vac}$$

confrg. on $\mathcal{M}\setminus\{x,y\}$

$$= \nu^2 \sum_{\tau} \underbrace{\left(\gamma_{(\uparrow,\downarrow,\tau)} - \gamma_{(\downarrow,\uparrow,\tau)}\right)}_{=0} \left(\prod \hat{a}^\dagger_{z\tau_z}\right) \Phi_{vac}$$

$\because$

$$\hat{C}_{u\downarrow}\hat{C}_{u\uparrow}\Phi = 0 \Rightarrow \gamma_{\sigma} = \gamma_{\sigma_{x\leftrightarrow y}} \text{ for } \forall \sigma$$

σ_x and σ_y are exchanged

$$\boxed{\text{repulsion in real space} \longrightarrow \text{"exchange interaction" in state space}}$$

using this repeatedly

$$\gamma_{\sigma} = \gamma_{\sigma'} \quad \text{if} \quad \sum_{x\in M} \sigma_x = \sum_{x\in M} \sigma'_x$$

$$\therefore \quad \Phi = \sum_{n=0}^{|M|} \underbrace{\alpha_n}_{\text{arbitrary}} (\hat{S}^-_{tot})^n \Phi_{\uparrow}$$

$S_{tot} = \frac{N}{2}$ and $(2S_{tot}+1)$ fold degenerate.

§ Some remarks

basic mechanism

multi-band structure

↓

restriction to the lowest band

not completly localized.

then

Coulomb repulsion in real space → repulsion in state space

Coulomb repulsion in real space → exchange interaction in state space

maybe robust (and realistic) ~~in some situations~~.

BUT

- $\hat{H}_{hop}$ and $\hat{H}_{int}$ are minimized simultaneously.

Although $[\hat{H}_{hop}, \hat{H}_{int}] \neq 0$, there is no real competition

- For $U=0$ the g.s. are highly degenerate and have

$$S_{tot} = 0, 1, \cdots, \frac{N}{2}$$

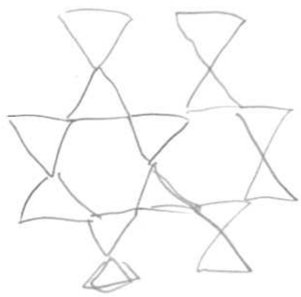
selected when $U>0$

The result is nontrivial and maybe physical, but is still easy

Mielke's result 91

the first flat-band ferromagnetism for the Hubbard model on the Kagomé lattice

No "fine-tuning"!



⟨Ferromagnetism in a non-singular Hubbard model⟩

- Nagaoka–Thouless ferromagnetism $U=\infty$
- flat-band ferromagnetism density of states $=\infty$

both are singular

ferromagnetism in models with nearly-flat band ?

plausible

also numerical results on stability (Kusakabe)

BUT difficult

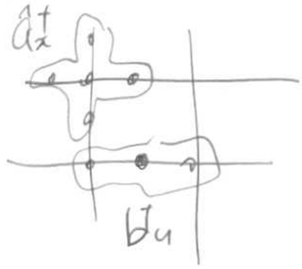
$U=0$ and probably for small U → Pauli para

$\hat{H}_{hop}$ and $\hat{H}_{int}$ cannot be minimized simultaneously!!

ferromagnetism is expected only for sufficiently large U

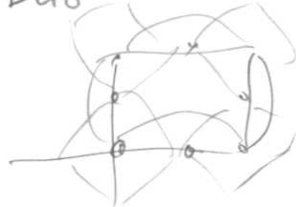
truly nonperturbative!

§ the model and main results



the same lattice,
the same a, b.
$s>0$, $t>0$

$$\hat{H}_{hop} = \underbrace{-s \sum_{\substack{x\in\mathcal{M} \\ \sigma=\uparrow,\downarrow}}{}' \hat{a}^\dagger_{x\sigma}\hat{a}_{x\sigma}}_{\text{new term}} + t \sum_{\substack{u\in\mathcal{O} \\ \sigma=\uparrow,\downarrow}}{}' \hat{b}^\dagger_{u\sigma}\hat{b}_{u\sigma}$$



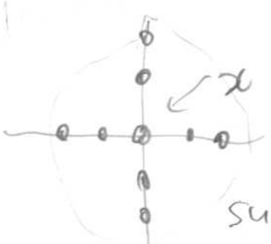
the lowest band is no longer flat for $s>0$.

<u>Theorem</u> (Tasaki 1995, 2003)

$N=|\mathcal{M}|$, t/s, U/s, $1/\nu$ sufficiently large

the g.s. have $S_{tot}=N/2$, and are non-degenerate apart from the trivial degeneracy.

<u>strategy of the proof</u> $\hat{H} = \sum'_{x\in\mathcal{M}} \hat{h}_x$ → crazy



$[\hat{h}_x, \hat{h}_y] \neq 0$ if $|x-y|\leq 2$.

minimize $\hat{h}_x$ simultaneously.

This (miraculously) works!

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

<u>Theorem</u> (Tasaki 1994, 1996)

translation operator

Let $E_{SW}(\mathbb{k}) = \min\{\langle\Phi, \hat{H}\Phi\rangle \mid \hat{S}^{(3)}_{tot}\Phi = \left(\frac{N}{2}-1\right)\Phi, \|\Phi\|=1,$
$\hat{\tau}_x[\Phi] = e^{i\mathbb{k}\cdot x}\Phi\}$

When t/s, U/s, t/U, $1/\nu$ suff. large

$$E_{SW}(\mathbb{k}) - E_{GS} \simeq \underbrace{4\nu^2 U \sum_{i=1}^{d} \left(\sin\frac{k_i}{2}\right)^2}_{\text{normal spin-wave excitation energy}}.$$

<u>strategy of the proof</u> rigorous perturbation. based on elementary linear algebra

119 pages

$$\boxed{\text{The first rigorous example of a non-singular itinerant electron system which exhibits "healthy" ferromagnetism.}}$$

<Metallic ferromagnetism>

the g.s. of the model with $N = |\mathcal{M}|$

$$\Phi_{\uparrow} = \left(\prod_{x \in \mathcal{M}} a^{\dagger}_{x\uparrow} \right) \Phi_{\mathrm{vac}} = \mathrm{const.} \left(\prod_{j=1}^{|\mathcal{M}|} d^{\dagger}_{j\uparrow} \right) \Phi_{\mathrm{vac}}$$


"particle" picture


"wave" picture.

← The lowest band is fully filled

probably a Mott insulator

metallic ferromagnetism

→ the same set of electrons contribute to magnetism and conduction.

expected in the same model with $0 \lneq \mathrm{const} \leq \dfrac{N}{|\mathcal{M}|} \lneq 1$

but the proof seems formidably difficult

$$\Phi_{\uparrow} = \left(\prod_{j=1}^{N} d^{\dagger}_{j\uparrow} \right) \Phi_{\mathrm{vac}}$$

ferro g.s.


← partially filled

= no simple particle pictures

electrons really behave as "waves"!

No hope of simultaneously minimizing local $\hat{h}_x$!!

Tanaka-Tasaki 2007.　　with $d \geq 2$

the first rigorous example of the Hubbard model exhibiting metallic ferromagnetism.

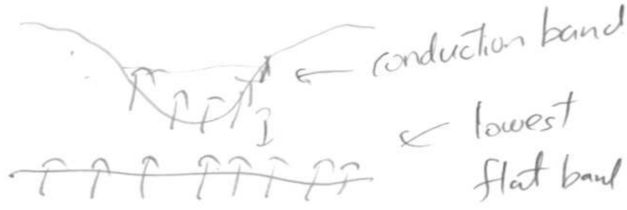
(but $U \nearrow \infty$, band gap $\nearrow \infty$)

- model　multi band system
- proof　short but a truly intricate math puzzle.

a starting point for further results ??

(NOT for the moment ...)

We are still working
on this problem
in
summer 2015



NO. last

DATE

<summary of Part3>

fundamental problem about the origin of ferromagnetism

quantum many-body effect of electrons

+

Coulomb interaction between electrons

"healthy" ferromagnetism

but an insulator
and
special classes of models.

metallic ferromagnetism OPEN!

ferromagnetism from many-body Schrödinger eq

WIDELY OPEN!!