Part 3

the origin of magnetism and the Hubbard model.

approaches from "constructive condensed matter physics"

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. $\downarrow$ 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 $\begin{cases} \text{mostly live on a site} = \text{atom} \\ \text{"hops" from a site to another} \end{cases}$

<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>

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

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

Spin operators

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

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

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

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

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

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

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

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

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

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

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

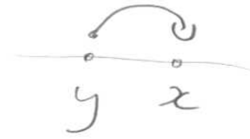
or

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

§ Hopping Hamiltonian

hopping amplitude $t_{xy} = t_{yx} \in \mathbb{R}$. ($t_{xx}$ on-site potential)

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



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

Single-electron energy eigenstates. → tightbinding 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 a "wave"

corresponding operator.

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

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

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

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

$$\because \sum_j \epsilon_j \hat{d}^\dagger_{j\sigma} \hat{d}_{j\sigma} = \sum_{j,x,y} \epsilon_j \psi^{(j)}_x (\psi^{(j)}_y)^* \hat{C}^\dagger_{x\sigma} \hat{C}_{y\sigma}$$

$$= \sum_{j,x,y,z} t_{xz} \underbrace{\psi^{(j)}_z (\psi^{(j)}_y)^*} \hat{C}^\dagger_{x\sigma} \hat{C}_{y\sigma}$$

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

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

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

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

→ 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, $\epsilon_j < \epsilon_{j+1}$ $(j = 1, 2, .., |\Lambda|-1)$

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 easy

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

(b) 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

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

on-site Coulomb interaction.

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

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

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

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

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

if $N \leq |\Lambda|$

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

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

$$\begin{array}{ccc} \uparrow & \downarrow & \uparrow \\ \bigcirc & \uparrow & \bigcirc \\ \downarrow & \uparrow & \downarrow \end{array}$$

g.s. are highly degenerate

$\hookrightarrow$ paramagnetism

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

electrons behave as "particles"

§ Hubbard model

$$\boxed{\begin{matrix} \hat{H} = \hat{H}_{hop} + \hat{H}_{int} \\ \text{"wave" "particle" dualism} \end{matrix}}$$

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

$\underline{U=0}$

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

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

$S_{Tot} = 0$

metallic if t_{xy} describes a single band.

$\underline{t_{xy}=0 \text{ or } U=\infty}$

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

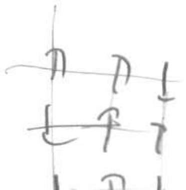
we can also write

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

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

spin configuration $\longleftrightarrow$ g.s.

highly degenerate g.s.



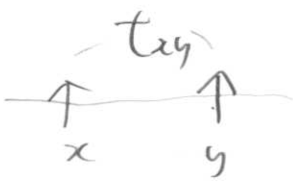
no electrons can hop

Mott insulator

§ Perturbation

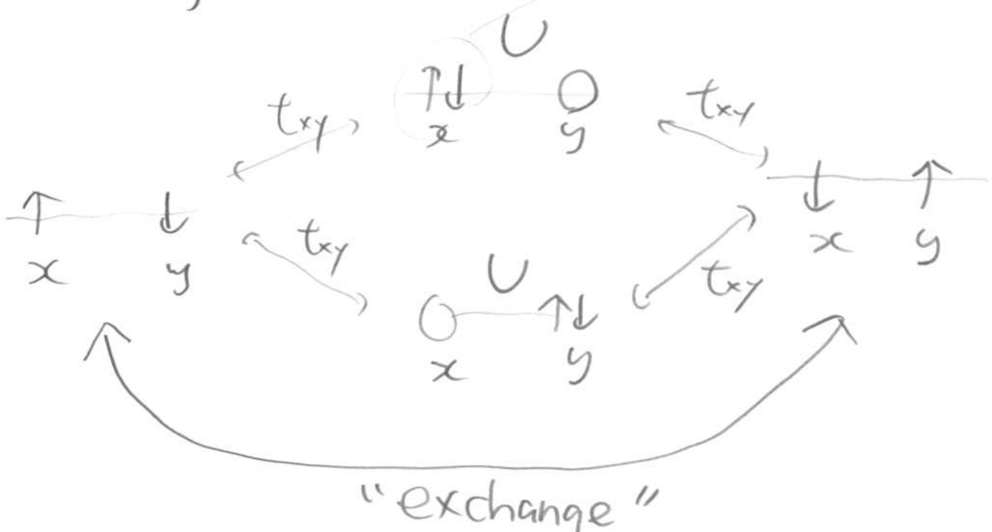
$|t_{xy}| \ll U$ → perturbation from the highly-degenerate g.s. Ψ^{Φ}.

2nd order pert. in t_{xy}



no hoppings!

singlet



the energy of the spin singlet is lowered.

effective Hamiltonian.

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

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 theorem

<u>Theorem</u> (Lieb 1989) $|\Lambda|$ even, $\Lambda = A \cup B$ (with $A \cap B = \phi$) and $t_{xy} \neq 0$ only when $x \in A, y \in B$ or $x \in B, y \in A$. Λ is connected by 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 non-degenerate apart from the trivial spin degeneracy.

the same as the g.s. of the Heisenberg AF

(but applies to any $U > 0$)

. But the <u>proof</u> is much harder than the Marshall-Lieb-Mattis theorem

not heavy but extremely clever
(fits in a PRL!)

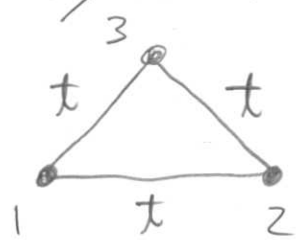
NO PROOF OF AF LRO

Hub-2** Fill <u>all gaps</u> in Lieb's PRL and compose an account readable to physicists and mathematicians.
(on the proof of the theorem which is in Japanese or in English)

⟨Towards ferromagnetism⟩

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

§ Toy model with three sites



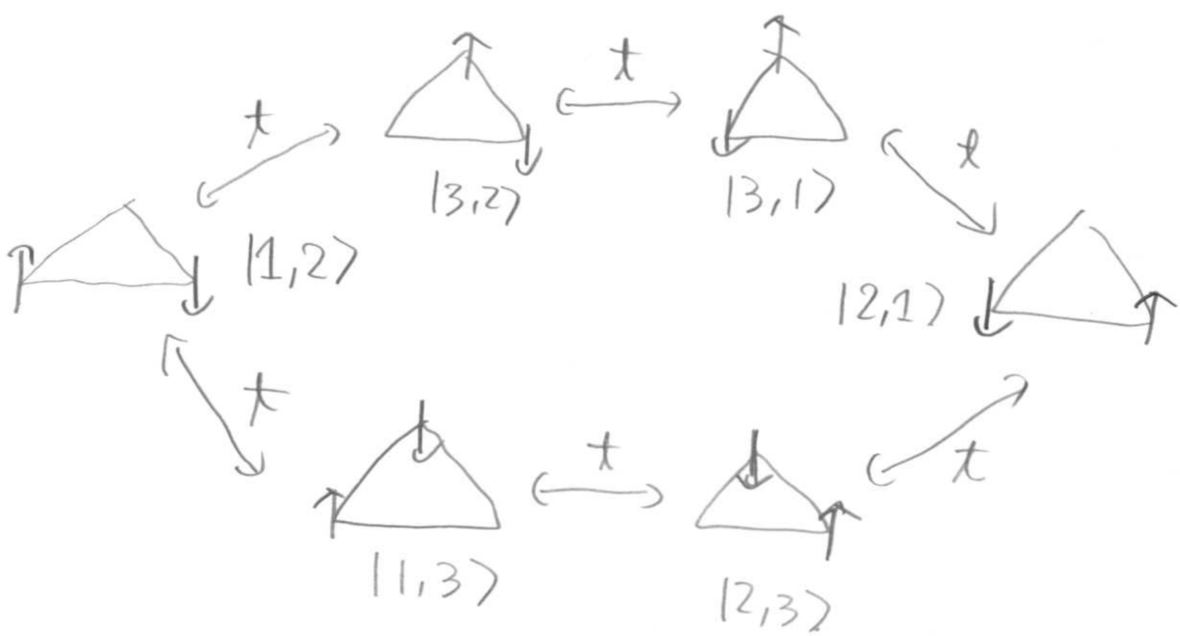
$N=2$

$U=\infty \rightarrow$ 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

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

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

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

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

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

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

<u>Hub-3</u> Prove this. (Use Perron-Frobenius)

<u>Hub-4</u> Examine the cases with $t_{xy}\in\mathbb{C}$, $(t_{xy})^*=t_{yx}$

skipped

§ Two interpretations of the toy model

motion of the "hole"

the "hole" moves along the triangle to realize ferro coupling

$\Downarrow$

Nagaoka-Thouless ferromagnetism

$\boxed{\begin{array}{l} U=\infty \\ N=|\Lambda|-1 \end{array}}$

a single hole!

"exchange interaction" on △

exchange

via the third site $\rightarrow$ ferro

$\Downarrow$

Flat-band ferromagnetism

section 4 ~~will be~~ was skipped

⟨Nagaoka-Thouless ferromagnetism⟩

§ Setting and the theorem

$N = |\Lambda| - 1$, $U \uparrow \infty \Rightarrow$ no double occupancies

only a single "hole" can move

$$\hat{H}_{\mathrm{hop}} = \sum_{\substack{x,y\\ \sigma}}{}' \, t_{xy} \hat{c}^\dagger_{x\sigma} \hat{c}_{y\sigma} \qquad \begin{array}{ccc} \uparrow & \downarrow & \uparrow \\ \uparrow & \bigcirc \leftarrow & \downarrow \\ \uparrow & \downarrow & \uparrow \end{array}$$

<u>Def</u>. The model satisfies the <u>connectivity condition</u> if for any $\mathcal{U}, D, \mathcal{U}', D' \subset \Lambda$ s.t. $\mathcal{U} \cap D = \phi$, $\mathcal{U}' \cap D' = \phi$, $|\mathcal{U}| = |\mathcal{U}'|$, $|D| = |D'|$, $|\mathcal{U}| + |D| = |\Lambda| - 1$, $\Psi_{\mathcal{U}', D'}$ is obtained from $\Psi_{\mathcal{U}, D}$ by allowed motion of the "hole".

- One gets all spin configurations by moving the hole.
  (example the three site model.)

- satisfied for most lattices in $d = 2$ or 3, but not for $d = 1$ chain.

<u>Theorem</u> (Thouless 65, Nagaoka 66, Tasaki 89)

$N = |\Lambda| - 1$, $U \uparrow \infty$, $t_{xy} \geq 0$, connectivity condition.

Then the g.s. have $S_{tot} = N/2$, and are nondegenerate apart from the trivial $(2S_{tot}+1)$ fold degeneracy.

$S_{tot} = N/2$ is the maximum possible spin.

$\downarrow$

saturated ferromagnetism

the first rigorous example of ferromagnetism in the Hubbard model.

But the single hole moves around the whole lattice and align the spins!

(not very realistic)

No results for models with multiple "holes"!

(ferromagnetism dissapears?)

§ Proof

basis states for $N=|\Lambda|-1$ and $U\uparrow\infty$

$\Psi_{x,\sigma}$ x: the position of the hole

$\sigma=(\sigma_y)_{y\in\Lambda\setminus\{x\}}$ spin config.

$$\Psi_{x,\sigma}=C_{x\uparrow}\Big(\prod_{y\in\Lambda}C^\dagger_{y,\sigma'_y}\Big)\Phi_{vac}$$

fix an ordering in Λ

$$\sigma'_y=\begin{cases}\sigma_y & y\neq x\\ \uparrow & y=x\end{cases}$$

then
$$\langle\Psi_{y,\tau},\hat{H}\Psi_{x,\sigma}\rangle=\begin{cases}-t_{xy} & \text{if } \tau=\sigma_{y\to x}\\ 0 & \text{otherwise}\end{cases}$$

i) $\exists$ g.s. with $S_{tot}=N/2$.

Take a normalized g.s. $\Phi_{GS}=\sum_{(x,\sigma)}\alpha_{x,\sigma}\Psi_{x,\sigma}$ coefficient

Let $\gamma_x=\sqrt{\sum_{\sigma}|\alpha_{x,\sigma}|^2}$ and.

$$\Phi_\uparrow=\sum_x\gamma_x\Psi_{x,(\uparrow)}$$ all up

now

$$E_{GS} = \langle \Phi_{GS}, \hat{H}\, \Phi_{GS} \rangle$$

$$= \sum_{\substack{(x,\sigma)\\(y,\tau)}} (\alpha_{y,\tau})^* \alpha_{x,\sigma} \langle \Phi_{y,\tau}, \hat{H}\, \Phi_{x,\sigma} \rangle$$

$$= -\sum_{x,y} t_{xy} \sum_{\sigma} (\alpha_{y,\sigma_{y\to x}})^* \alpha_{x,\sigma}$$

$$\geq -\sum_{x,y} t_{x,y} \sqrt{\sum_{\tau} |\alpha_{y,\tau}|^2 \sum_{\sigma} |\alpha_{x,\sigma}|^2}$$

$$= -\sum_{x,y} t_{x,y}\, \gamma_x \gamma_y$$

$$= \sum_{x,y} \gamma_x \gamma_y \langle \Phi_{y,(\uparrow)}, \hat{H}\, \Phi_{x,(\uparrow)} \rangle$$

$$= \langle \Phi_{\uparrow}, \hat{H}\, \Phi_{\uparrow} \rangle$$

So $\Phi_{\uparrow}$ is also a g.s.

ii) g.s. are unique

fix $S^{(3)}_{Tot} = \sum_{x} \sigma_x$

then all $\Phi_{x,\sigma}$ are connected.

PF theorem says that the g.s. in this sector is unique. But it must be

$$(\hat{S}^{-}_{Tot})^{\circ}\, \Phi_{\uparrow}$$

//

ferro g.s. in bulk?

⟨Flat-band ferromagnetism⟩

1st rigorous example

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

↕ more than 25 years!

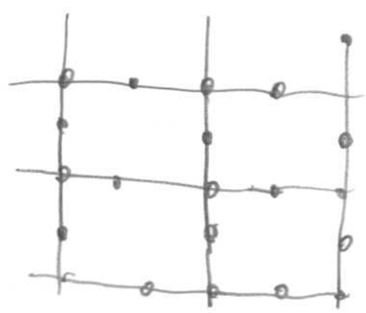
flat-band ferro Mielke 91, Tasaki 92. — $\boxed{D=\infty}$ (density of state)

$\left(\begin{array}{c}\text{Stoner criterion} \\ UD \text{ large} \\ \downarrow \\ \text{ferro}\end{array}\right)$ ← extremely heuristic

§ 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 $\mathcal{M}$
$\Downarrow$
$u, v, \ldots$



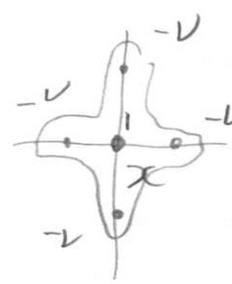
$$\Lambda = \mathcal{M} \cup \mathcal{O}$$

↑ decorated hyper cubic lattice

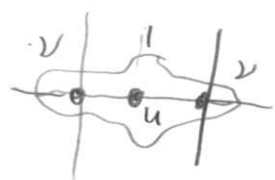
fix $\nu > 0$

fermion operators

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



a-state

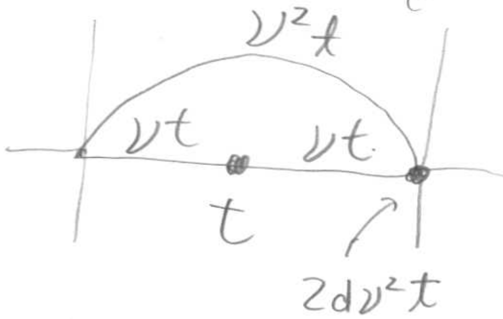


b-state

then $t > 0$

we let $\hat{H}_{hop} = t \sum_{\substack{u \in \mathcal{O} \\ \sigma = \uparrow, \downarrow}}' \hat{b}^{\dagger}_{u,\sigma} b_{u,\sigma} = \sum_{\substack{x,y \\ \sigma}}' t_{xy} c^{\dagger}_{x\sigma} c_{y\sigma}$

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



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.

§ Special properties of the model

- {all the a-states plus all the b-states} form a complete basis (for single-electron states)

- $\{\hat{a}^\dagger_{x\sigma}, \hat{b}_{u\tau}\} = 0$ for $\forall x, u, \sigma, \tau$.

- $$\{\hat{a}^\dagger_{x\sigma}, \hat{a}_{y,\sigma}\} = \begin{cases} 1 + 2d\nu^2 & x = y \\ \nu^2 & |x-y| = 1 \\ 0 & \text{otherwise.} \end{cases}$$

$\therefore$

$\hat{H}_{hop} \geq 0$, $\hat{H}_{hop}\Phi_{vac} = 0$, $[\hat{H}_{hop}, \hat{a}^\dagger_{x,\sigma}] = 0$ for $\forall x, \sigma$

So $\hat{H}_{hop}\,\overbrace{\hat{a}^\dagger_{x,\sigma}\Phi_{vac}}^{\text{g.s. for } N=1} = 0$ for $\forall x, \sigma$.

the single-electron ground states are $\overbrace{|\mathcal{M}|}^{L^d}$-fold degenerate!

- single-electron energy spectrum

→ flat-band

||

the result of (artificial) "fine-tuning".

§ Proof of the theorem

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

1) a g.s.

Let $\Phi_{\uparrow} = \left(\prod_{x \in \mathcal{M}_1} a^{\dagger}_{x\uparrow} \right) \Phi_{vac}$

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

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

other g.s.?

2) general g.s.

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

$$\hat{H}_{hop} = t \sum_{u,\sigma}{}' \hat{b}^{\dagger}_{u\sigma} \hat{b}_{u\sigma} \rightarrow \hat{b}_{u\sigma}\Phi = 0 \quad \text{for } {}^{\forall}u, \sigma \qquad ①$$

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

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

①, ② detailed conditions

• Spin system representation

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 $x\in\Lambda$

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

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

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

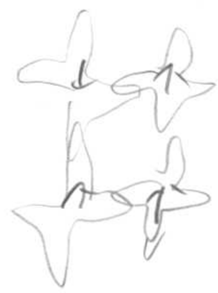
② ⇒ $\alpha_{\mathcal{U},\mathcal{D}} \neq 0$ only when $\mathcal{U}\cap\mathcal{D}=\phi$.

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

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

So we get the spin-system rep.

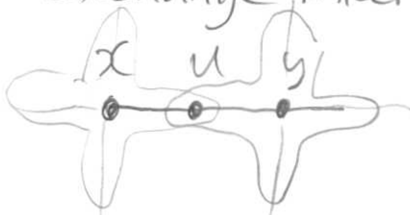
ひでー⊗.



$$\Phi = \sum_{\boldsymbol{\sigma}} \gamma_{\boldsymbol{\sigma}} \Big(\underbrace{\prod_{x \in \mathcal{M}}}_{\uparrow \text{ fixed ordering}} \hat{a}^{\dagger}_{x\sigma_x} \Big) \Phi_{\text{vac}}$$

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

- exchange interaction



$\hat{a}^{\dagger}$'s other than x, y

$$\hat{c}_{u\downarrow} \hat{c}_{u\uparrow} \hat{a}^{\dagger}_{x\sigma} \hat{a}^{\dagger}_{y\sigma'} (\cdots) \Phi_{\text{vac}} = \begin{cases} \nu^2 (\cdots) \Phi_{\text{vac}} & \sigma = \uparrow, \sigma' = \downarrow \\ -\nu^2 (\cdots) \Phi_{\text{vac}} & \sigma = \downarrow, \sigma' = \uparrow \\ 0 & \text{otherwise.} \end{cases}$$

thus

$$\hat{c}_{u\downarrow} \hat{c}_{u\uparrow} \Phi = 0 \Rightarrow \gamma_{\boldsymbol{\sigma}} = \gamma_{\boldsymbol{\sigma}_{x \leftrightarrow y}}$$

σ_x and σ_y are exchanged

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

↓
using this repeatedly,

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

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

$S_{tot} = \frac{N}{2}$, 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

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

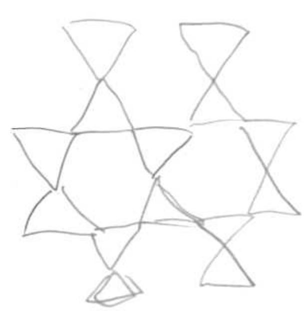
selected when $U>0$

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"!



DATE

⟨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 !

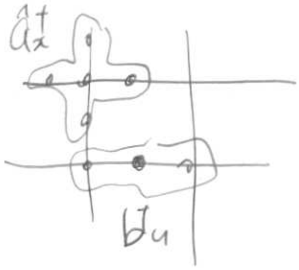
↓

ferromagnetism is expected only for sufficiently large U

↓

truly nonperturbative!

§ the model and main results

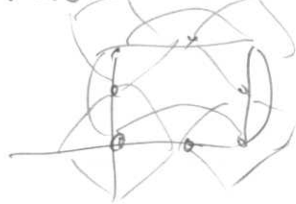


the same lattice,

the same a, b.

$s>0,\ t>0$

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



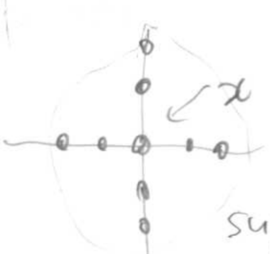
the lowest band is no longer flat for $s>0$

Theorem (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.

strategy of the proof $\hat{H} = \sum_{x\in\mathcal{M}}{}' \hat{h}_x$ → crazy



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

minimize $\hat{h}_x$ simultaneously.

This (miraculously) works!

↑↑↓↑↑?↑

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

translation operator

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

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

$$E_{SW}(\mathbb{k}) - E_{GS} \simeq 4\nu^2 U \sum_{i=1}^{d} \left(\sin\frac{k_i}{2}\right)^2.$$

normal spin-wave excitation energy

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

119 pages

> The first rigorous example of a non-singular itinerant electron system which exhibits "healthy" ferromagnetism.

⟨Metallic ferromagnetism⟩

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

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

"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 $0 \lneq \text{const} \leq \frac{N}{|\mathcal{M}|} \lneq 1$

but the proof seems formidably difficult

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

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.

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.

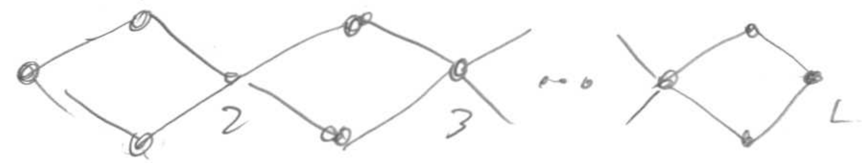
a starting point for further results ??

(NOT for the moment ...)

§ An (incomplete) approach to metallic ferromagnetism

(Tanaka, Tasaki unpublished)

$\mathcal{M} = \{1, 2, \ldots, L\}$ open chain



Θ, Θ' the sets of sites between x and $x+1$

(Sekizawa 2003)

$\Lambda = \mathcal{M} \cup \Theta \cup \Theta'$

$\nu > 0$

$x \in \mathcal{M}$

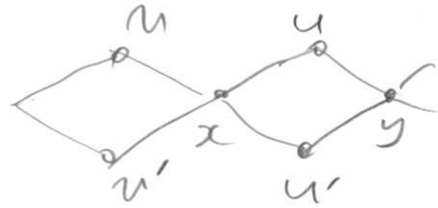
$$\hat{a}_{x\sigma} = \text{const.}\left\{\hat{c}_{x\sigma} + \nu\{\hat{c}_{u\sigma} - \hat{c}_{u'\sigma} + \hat{c}_{v,\sigma} + \hat{c}_{v'\sigma}\}\right\}$$

$u \in \Theta$

$$\hat{b}_{u\sigma} = \hat{c}_{u\sigma} - \nu\{\hat{c}_{x\sigma} + \hat{c}_{y\sigma}\}$$

$u' \in \Theta$

$$\hat{b}_{u'\sigma} = \hat{c}_{u'\sigma} + \nu\{\hat{c}_{x\sigma} - \hat{c}_{y\sigma}\}$$



then $\{\hat{a}^\dagger_{x\sigma}, \hat{a}_{y\sigma}\} = \delta_{xy}$ normal!

$\{\hat{a}^\dagger, \hat{b}\} = 0$

$t>0,\ s>0$

$$\begin{cases} \hat{H}_{hop} = -t \displaystyle\sum_{\substack{x,y\in M \\ (|x-y|=1)}} \sum_{\sigma=\uparrow,\downarrow} \hat{a}^\dagger_{x\sigma}\hat{a}_{y\sigma} + s \sum_{\substack{\tilde{u}\in\Theta\cup\Theta' \\ \sigma=\uparrow,\downarrow}} \hat{b}^\dagger_{\tilde{u}\sigma}\hat{b}_{u\sigma} \\ \hat{H}_{int} = U \displaystyle\sum_{z\in\Lambda} \hat{n}_{z\uparrow}\hat{n}_{z\downarrow} \end{cases}$$

$$\hat{H} = \hat{H}_{hop} + \hat{H}_{int}$$

$$N \lneqq |M|$$

We let $s\uparrow\infty$, $U\uparrow\infty$ (although we don't want to...)

then any Φ s.t. $\langle\Phi, \hat{H}\Phi\rangle < \infty$ satisfies

$$\hat{b}_{\tilde{u}\sigma}\Phi = 0 \quad \forall\tilde{u}\in\Theta\cup\Theta',\ \sigma=\uparrow,\downarrow \qquad \hat{c}_{z\downarrow}\hat{c}_{z\uparrow}\Phi = 0 \quad \forall z\in\Lambda$$

(as in the flat-band case)

then

$$\boxed{\Phi = \sum_{C\subset M} \sum_{\sigma \text{ on } C} \alpha_{C,\sigma} \left(\prod_{x\in C} a^\dagger_{x,\sigma(x)}\right)\Phi_{vac}}$$

+ in each connected component of C, all the spins are coupled ferromagnetically (to form the highest spin state)

The g.s. is exactly the same as that of the ferromagnetic t-J model on Λ with

$$\hat{H}_{\mathrm{eff}} = -\sum_{\substack{x,y\in\Lambda \\ (|x-y|=1)}}' \sum_{\sigma=\uparrow,\downarrow}' \hat{a}^{\dagger}_{x\sigma} \hat{a}_{y\sigma}$$

$$- J \sum_{\substack{x,y\in\Lambda \\ (|x-y|=1)}}' \left\{ \hat{S}_x \cdot \hat{S}_y - \frac{\hat{n}_x + \hat{n}_{x+1}}{4} \right\}$$

(defined in terms of $\hat{a}$'s)

and $J \uparrow \infty$.

<u>$d=1$</u> Perron-Frobenius
↓
the g.s. exhibits metallic ferro.
but 1D is easy and less interesting

<u>$d \geq 2$</u> NO RESULTS !! (unless $|\Lambda| \geq N > |\Lambda| - 2d$)
→ C is connected !

indeed we expect no ferro for $\dfrac{N}{|\Lambda|} \ll 1$.

(better results if there are diagonal hoppings)

$\boxed{\text{We still miss something essential !}}$

<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!!