SU(N) Hubbard 模型における厳密な結果

桂 法称 (東京大学・物理学専攻)

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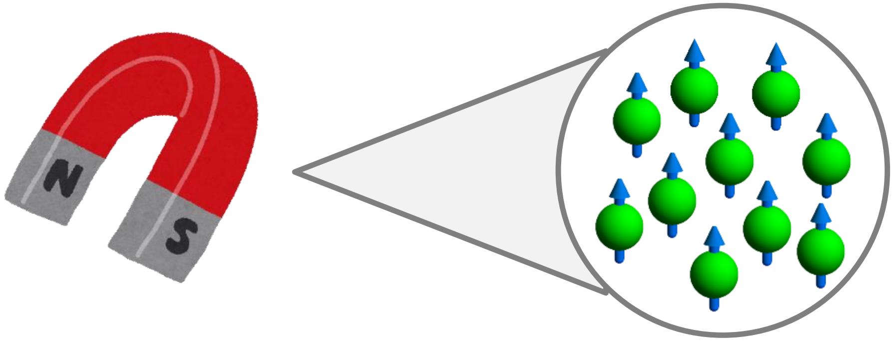
Outline

1. Introduction
   - 磁性と SU(2) Hubbard 模型
   - 冷却原子系と SU(N) Hubbard 模型
2. 強磁性についての厳密な結果
3. 引力Hubbard模型についての厳密な結果
4. Summary

磁石の起源

強磁性はどのような機構で発現するの?



巨視的な数のスピン
(電子が担う)が一斉に同じ
方向に揃うことによる

But why?

■ スピン間に働く相互作用

- 双極子相互作用 $$U_{\mathrm{dip}}(\boldsymbol{r}) \propto -\frac{\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2}{r^3} + 3\frac{(\boldsymbol{\mu}_1 \cdot \hat{r})(\boldsymbol{\mu}_2 \cdot \hat{r})}{r^3}$$

Usually, too small (< 1K) to explain transition temperatures…

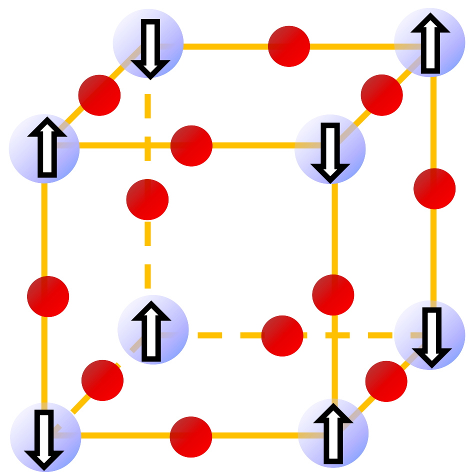
- 交換相互作用

$$H_{\mathrm{int}} = J\boldsymbol{S}_i \cdot \boldsymbol{S}_j$$ ($\boldsymbol{S}_i$: spin at site *i*)

直接交換(direct exchange): $J < 0$ → 強磁性的 (FM)
超交換(super-exchange): $J > 0$ → 反強磁性的 (AFM)

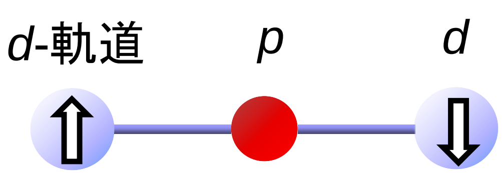
Magnetism in reality

■ 金森-Goodenough 規則

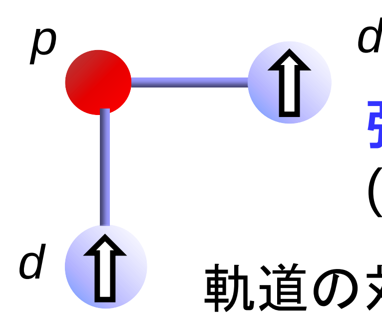


磁性イオン (cations) の間に
直接の相互作用はなく、陰イオン
(anions) を介して相互作用する

• 単純な例 (軌道秩序は無視)



磁性イオン間に
反強磁性相互作用



強磁性相互作用
(except for d^5.)

軌道の対称性に基づいた議論

より単純なモデルにおいて厳密に強磁性を証明できない?

SU(2) Hubbard模型

固体中の相関電子系を記述する単純な格子模型

Hubbard, *Proc. Roy. Soc. A* **276**, 238 (1963)

Electron correlations in narrow energy bands

By J. Hubbard

Theoretical Physics Division, A.E.R.E., Harwell, Didcot, Berks

(*Communicated by B. H. Flowers, F.R.S.—Received* 23 *April* 1963)

Hubbard
Kanamori, Gutzwiller

- 原論文でのハミルトニアン

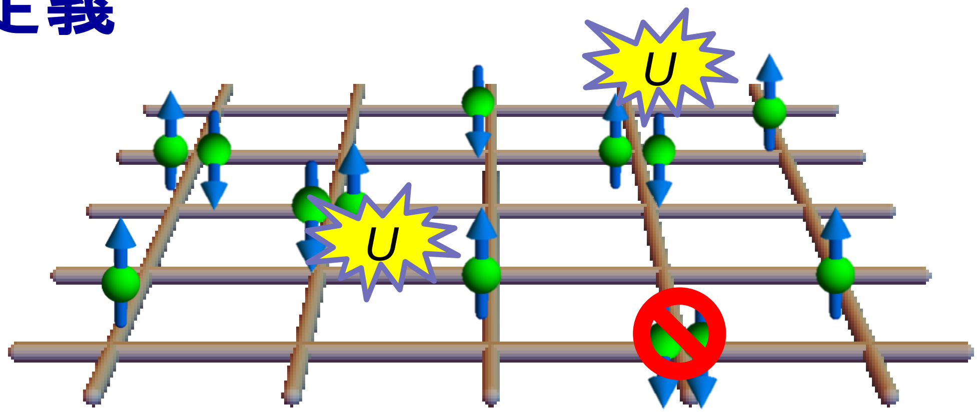
made, then the Hamiltonian of (6) becomes

$$H = \sum_{i,j} \sum_{\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \tfrac{1}{2} I \sum_{i,\sigma} n_{i\sigma} n_{i,-\sigma} - I \sum_{i,\sigma} \nu_{ii} n_{i\sigma},$$

where $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. From (9), $\nu_{ii} = N^{-1} \sum_{\mathbf{k}} \nu_{\mathbf{k}} = \frac{1}{2} n$, so the last term

SU(2) Hubbard模型: 定義

■ Setup



- Λ : finite lattice
- $x, y, \ldots$: site index
- $\sigma = \uparrow$ or $\downarrow$: spin index
- $c^\dagger_{x,\sigma}$ $(c_{x,\sigma})$: creation (annihilation) operator
  $\{c_{x,\sigma}, c_{y,\sigma'}\} = \{c^\dagger_{x,\sigma}, c^\dagger_{y,\sigma'}\} = 0, \quad \{c_{x,\sigma}, c^\dagger_{y,\sigma'}\} = \delta_{x,y}\delta_{\sigma,\sigma'}$

$\bullet^\dagger(\text{phys}) = \bullet^*(\text{math})$

- $n_{x,\sigma} := c^\dagger_{x,\sigma} c_{x,\sigma}$: number operator

■ Hamiltonian

Hopping matrix

$$H = H_{\text{hop}} + H_{\text{int}}$$

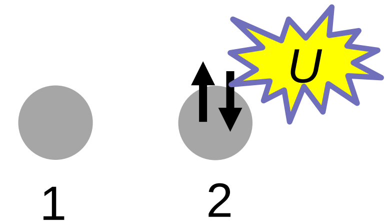
Hopping term $\quad H_{\text{hop}} = \sum_{\sigma=\uparrow,\downarrow} \sum_{x,y\in\Lambda} t_{x,y} c^\dagger_{x,\sigma} c_{y,\sigma}$

On-site Coulomb $\quad H_{\text{int}} = U \sum_{x\in\Lambda} n_{x,\uparrow} n_{x,\downarrow}$

SU(2) 不変性をもつ

H_{hop}とH_{int}は交換しない…

超交換相互作用の「導出」



■ 2サイトのHubbard模型

- Hamiltonian

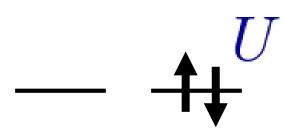
$$H = -t \sum_{\sigma=\uparrow,\downarrow} (c^\dagger_{1,\sigma} c_{2,\sigma} + c^\dagger_{2,\sigma} c_{1,\sigma}) + U \sum_{i=1,2} n_{i,\uparrow} n_{i,\downarrow}$$

- half-filling ($N_\mathrm{e} = 2$) での二次摂動, $U \gg t$

Basis states: $|\sigma_1, \sigma_2\rangle = c^\dagger_{1,\sigma_1} c^\dagger_{2,\sigma_2} |\mathrm{vac}\rangle$

$t = 0$

Pauli's exclusion



$$\begin{array}{cc} \begin{pmatrix} 0 & & & \\ & -\frac{2t^2}{U} & +\frac{2t^2}{U} & \\ & +\frac{2t^2}{U} & -\frac{2t^2}{U} & \\ & & & 0 \end{pmatrix} & \begin{array}{c} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{array} \end{array}$$

$$\boxed{H_\mathrm{eff} = \frac{4t^2}{U}\left(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 - \frac{1}{4}\right)}$$

$$S_i^\alpha = \frac{1}{2}\sigma_i^\alpha$$

交換相互作用の起源 = 電子間相互作用!

反強磁性相互作用を説明。強磁性相互作用についてはどうか?

「強磁性を示す」とは？

■ SU(2) Hubbard模型の対称性

- 総電子数 $N_\mathrm{e} := \sum_{x\in\Lambda}(n_{x,\uparrow}+n_{x,\downarrow})$
- 全スピン演算子

$$S^a_\mathrm{tot} := \sum_{x\in\Lambda} S^a_x \quad (a=\mathrm{x},\mathrm{y},\mathrm{z})$$

各サイトのスピン

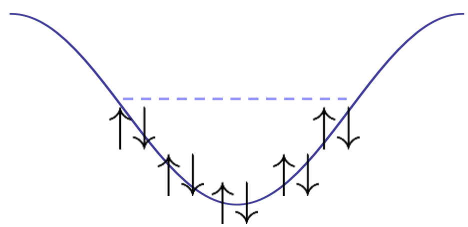
$$S^a_x := \sum_{\sigma,\tau} c^\dagger_{x,\sigma}\frac{\sigma^a_{\sigma,\tau}}{2}c_{x,\tau}$$

- ハミルトニアン *H* は、これらと交換 $[H, N_\mathrm{e}] = [H, S^a_\mathrm{tot}] = 0$
- *H* は次の変換で不変 $c_{x,\sigma} \to \tilde{c}_{x,\sigma} = \sum_{\tau=\uparrow,\downarrow}\mathcal{U}_{\sigma,\tau}c_{x,\tau}, \quad \mathcal{U}\in\mathrm{U}(2)$

■ 強磁性状態

- *H* の固有状態は、$(\boldsymbol{S}_\mathrm{tot})^2, S^\mathrm{z}_\mathrm{tot}$ の同時固有状態にとれる
- 強磁性状態は、N_e を固定した部分空間で $(\boldsymbol{S}_\mathrm{tot})^2$ が最大の状態
- 以下、基底状態が強磁性状態のみとなるとき、強磁性を示すという

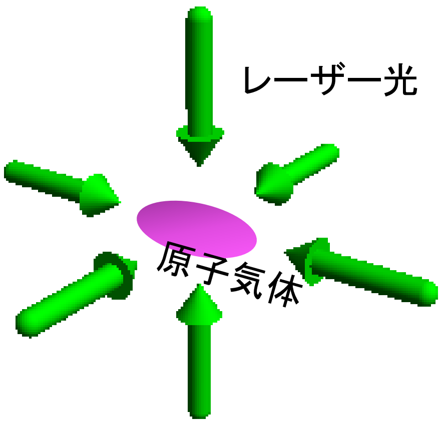
NOTE) 相互作用がないと基底状態はシングレット

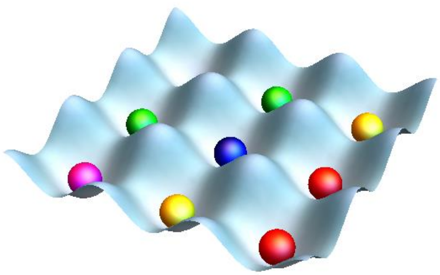


SU(*N*) Hubbard模型: motivation

■ 光格子系

レーザー光の定在波の腹・節
による人工的な結晶格子
原子を閉じ込めることができる

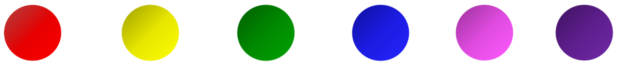




■ *N*成分フェルミオン系

核スピンの自由度をもつ原子

^{173}Yb
核スピン I = 5/2, 磁気副準位 σ = -5/2, -3/2, -1/2, 1/2, 3/2, 5/2



^{87}Sr
核スピン I = 9/2 → N=10成分系

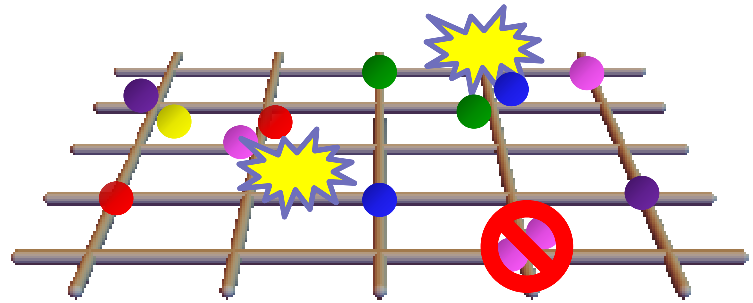
核スピンは電子スピンと分離 → SU(*N*) 対称な相互作用

SU(6) Hubbard模型の実験的実現(京大・高橋グループ)
Taie *et al*., *Nature Physics*, **8**, 825 (2012)
強相関系の量子シミュレーション

SU(N) Hubbard模型: 定義

■ Setup

- Λ : finite lattice
- $x, y, \ldots$: site index
- $\alpha = 1, 2, \ldots, N$: color index
- $c^\dagger_{x,\alpha}$ $(c_{x,\alpha})$: creation (annihilation) operator
  $\{c_{x,\alpha}, c_{y,\beta}\} = \{c^\dagger_{x,\alpha}, c^\dagger_{y,\beta}\} = 0, \quad \{c_{x,\alpha}, c^\dagger_{y,\beta}\} = \delta_{x,y}\delta_{\alpha,\beta}$
- $n_{x,\alpha} := c^\dagger_{x,\alpha} c_{x,\alpha}$: number operator
- $|\mathrm{vac}\rangle$: vacuum such that $c_{x,\alpha}|\mathrm{vac}\rangle = 0 \ \forall x, \alpha$ and $\langle \mathrm{vac}|\mathrm{vac}\rangle = 1$



■ Hamiltonian $\quad H = H_{\mathrm{hop}} + H_{\mathrm{int}}$

- Hopping term

$$H_{\mathrm{hop}} = \sum_{\alpha=1}^{N} \sum_{x,y\in\Lambda} t_{x,y} c^\dagger_{x,\alpha} c_{y,\alpha}$$

- Interaction term $\quad H_{\mathrm{int}} = U \displaystyle\sum_{1\le\alpha<\beta\le N} \sum_{x\in\Lambda} n_{x,\alpha} n_{x,\beta}$

Cazalilla *et al*., *NJP*, **11** (2009)
Gorshkov *et al*., *Nat. Phys*. **6** (2010)

SU(N) 強磁性状態とは？

■ 模型の対称性

- Total fermion num. $F_{\mathrm{tot}} := \sum_{\alpha=1}^{N} \sum_{x\in\Lambda} n_{x,\alpha}$
- Generators

$$F^{\alpha,\beta} := \sum_{x\in\Lambda} c^{\dagger}_{x,\alpha} c_{x,\beta}$$

$F^{\alpha,\alpha}$ の固有値を F_α で表す

- ハミルトニアンはこれらと交換 $[H, F^{\alpha,\beta}] = 0$

F_{tot} を固定した空間でSU(N) 対称性

- H は以下の変換で不変

$$c_{x,\alpha} \to \tilde{c}_{x,\alpha} = \sum_{\beta=1}^{N} \mathcal{U}_{\alpha,\beta} c_{x,\beta}, \quad \mathcal{U} \in \mathrm{U}(N)$$

■ SU(N)強磁性状態

- Hは、$(F_1, \cdots, F_N)$ で指定される部分空間ごとにブロック対角
- 異なる部分空間に属するHの縮退したエネルギー固有状態は、$F^{\alpha,\beta}(\alpha \neq \beta)$ の作用により関係付いている
- 強磁性状態は、F_{tot} を固定した部分空間で2次のCasimirの固有値が最大の状態

$$C_2 = \frac{1}{2}\left(\sum_{\alpha,\beta=1}^{N} F^{\alpha,\beta} F^{\beta,\alpha} - \frac{(F_{\mathrm{tot}})^2}{N} \right)$$

Outline

1. Introduction

2. 強磁性についての厳密な結果

- 長岡強磁性
- 平坦バンド強磁性

3. 引力Hubbard模型についての厳密な結果

4. Summary

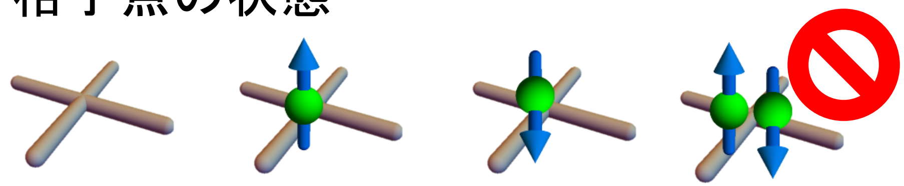
強磁性 (FM) についての厳密な結果

ある種のクラスのHubbard模型については、基底状態が強磁性を示す (unique g.s. が強磁性状態である)ことを証明できる

	SU(2) Hubbard	SU(*N*) Hubbard
Nagaoka FM	Nagaoka, PR **147** (1966) Tasaki, PRB **40** (1989)	Katsura & Tanaka, PRA **87** (2013) Bobrow *et al.*, PRB **98** (2018)
Flat-band FM	Mielke, J. Phys. A **A24** (1991) Tasaki, PRL **69** (1992)	Liu et al., Sci. Bull. **64** (2019) Tamura & Katsura, PRB **100** (2019)
Nearly flat-band FM	Tasaki, PRL **75** (1995) Tasaki, CMP **242** (2003)	Tamura & Katsura, PRB **100** (2019) Tamura & Katsura, JST **182** (2021)
General theory	Mielke, PLA **174** (1995) Mielke, JPA **32** (1999)	Tamura & Katsura, in preparation (Tamura-san’s talk)

長岡強磁性

- 反発力(U)無限大の極限
  - 各格子点の状態



格子点に2つ電子
がいる配置を無視できる

- 定理 (Nagaoka, 1965; Tasaki, 1989)

仮定

1. $t_{x,y} \geq 0, \ U = \infty$
2. 総電子数 $N_{\mathrm{e}} = |\Lambda| - 1$
3. 格子 Λ は二部連結グラフ

Then the ground state of the SU(2) Hubbard model has the maximum total spin $S_{\max} = (|\Lambda| - 1)/2$ and unique up to the trivial |Λ|-fold degeneracy.

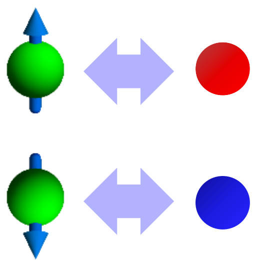
Eigenvalue of $(\boldsymbol{S}_{\mathrm{tot}})^2$:

$$\frac{N_{\mathrm{e}}}{2}\left(\frac{N_{\mathrm{e}}}{2} + 1\right)$$

特殊だが、ハバード・モデルから強磁性を厳密に示した最初の例！

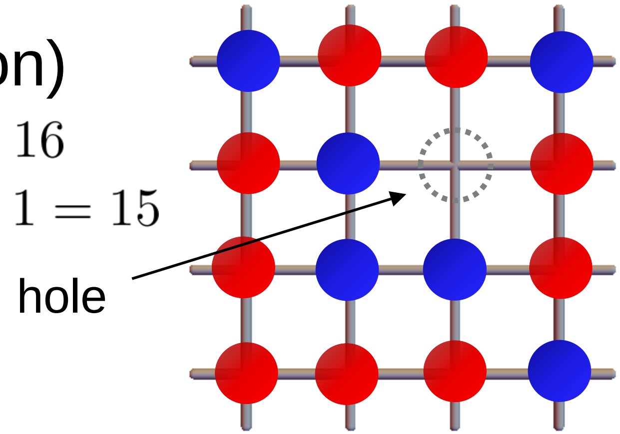
証明のアウトライン

■ 連結性条件 (connectivity condition)



$$\mathrm{Ex.)}\ |\Lambda| = 16$$
$$N_{\mathrm{e}} = |\Lambda| - 1 = 15$$

ホールを動かすことで
任意の配置を実現できる

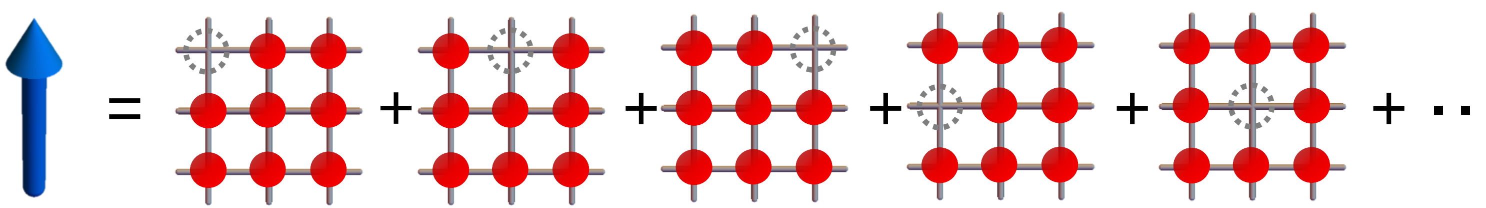


■ Perron-Frobenius (PF) の定理

- Basis states $|i, \boldsymbol{\sigma}\rangle = (-1)^i c^\dagger_{1,\sigma_1} \cdots c^\dagger_{i-1,\sigma_{i-1}} c^\dagger_{i+1,\sigma_{i+1}} \cdots c^\dagger_{|\Lambda|,\sigma_{|\Lambda|}} |\mathrm{vac}\rangle$

  この基底では、hopping term H_{hop} のすべての
  非対角要素はゼロ以下 $\langle i, \boldsymbol{\sigma} | H_{\mathrm{hop}} | j, \boldsymbol{\tau} \rangle \leq 0$

- 連結性条件を満たす場合、PF定理から、total S^z を固定した部分空間では基底状態は unique と言える



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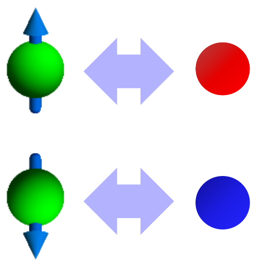

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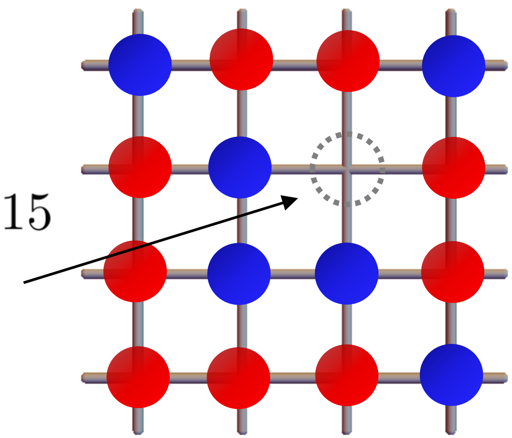

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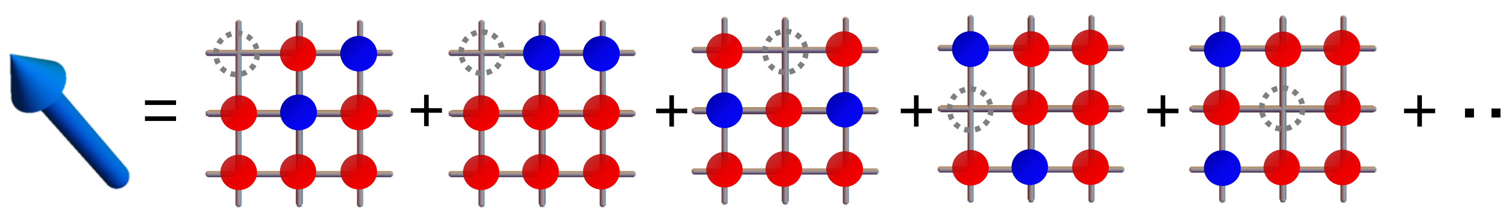
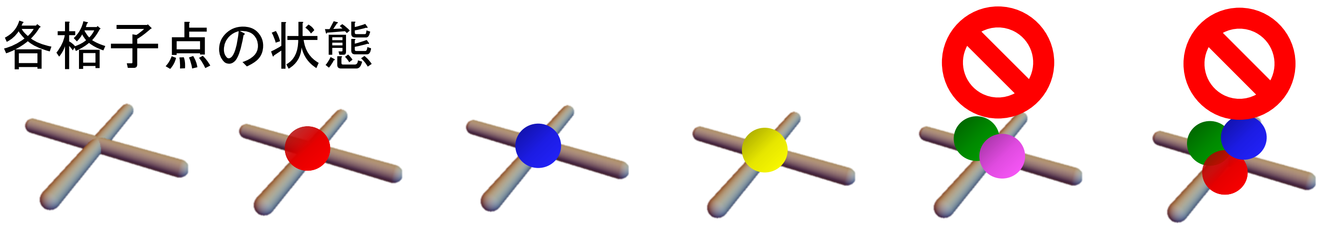


What about SU(*N*)?

■ 反発力(*U*)無限大の極限

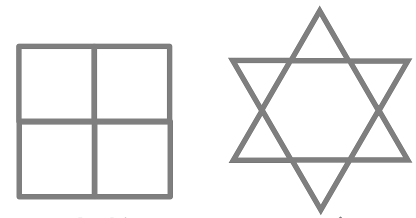
- 各格子点の状態



■ 定理 (Katsura & Tanaka, 2012)

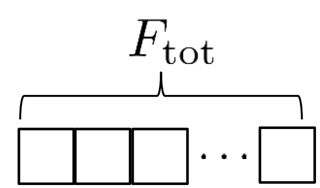
仮定

1. $t_{x,y} \geq 0,\ U = \infty$
2. 総フェルミオン数　$F_{\mathrm{tot}} = |\Lambda| - 1$
3. 連結性条件を満たす



> Then the ground state of the SU(*N*) Hubbard model is SU(*N*) ferromagnetic and unique up to the trivial d_{deg}-fold degeneracy.

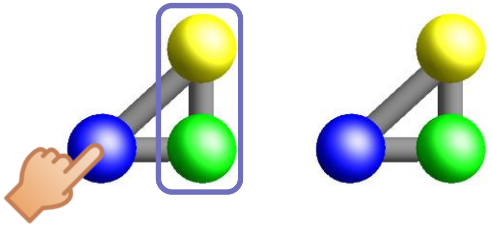
$$d_{\mathrm{deg}} = \binom{F_{\mathrm{tot}} + N - 1}{F_{\mathrm{tot}}}$$



- 2次のCasimir演算子の値が最大の状態
- Cf.) Miyashita, Ogata & De Raedt, *PRB* **80**, 174422 (2009)

証明のアウトライン

- 連結性条件
  - パズドラと非常に似ている
  - ホール ~ タッチしたドロップ
  - 局所的な互換



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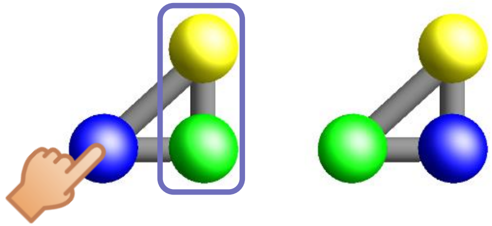

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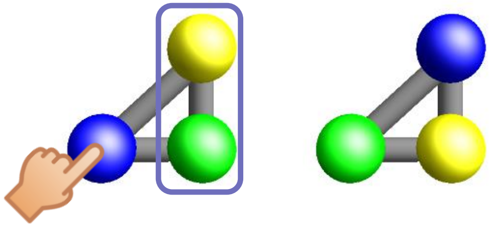

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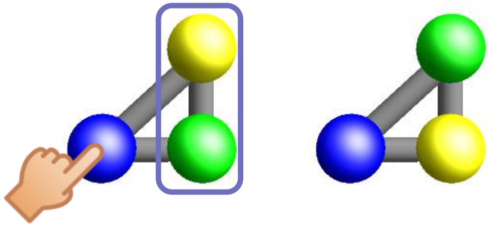

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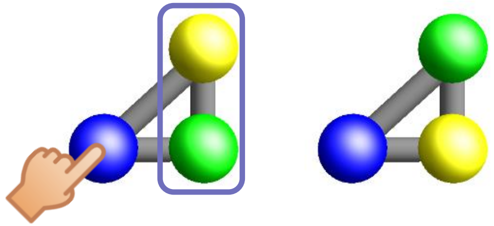

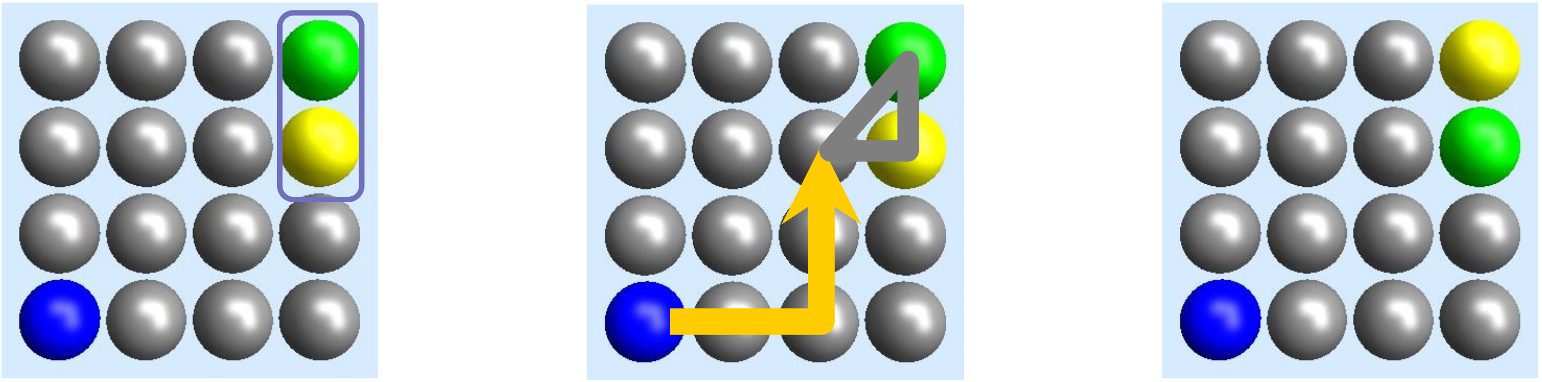

証明のアウトライン

■ 連結性条件

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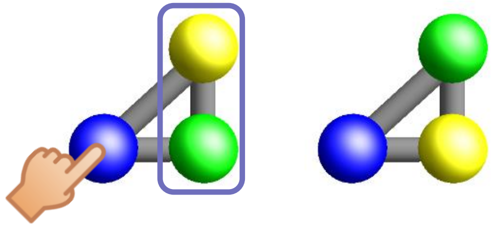

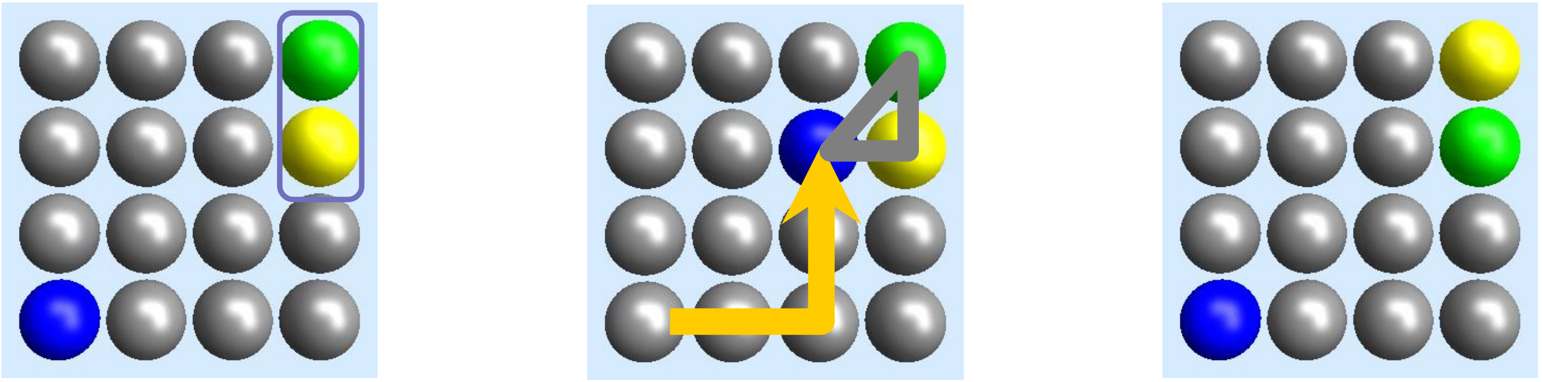

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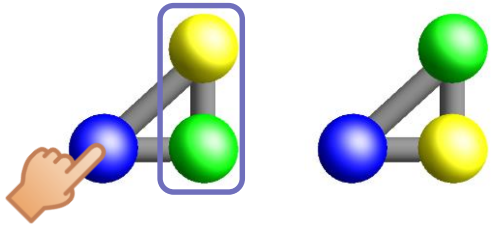

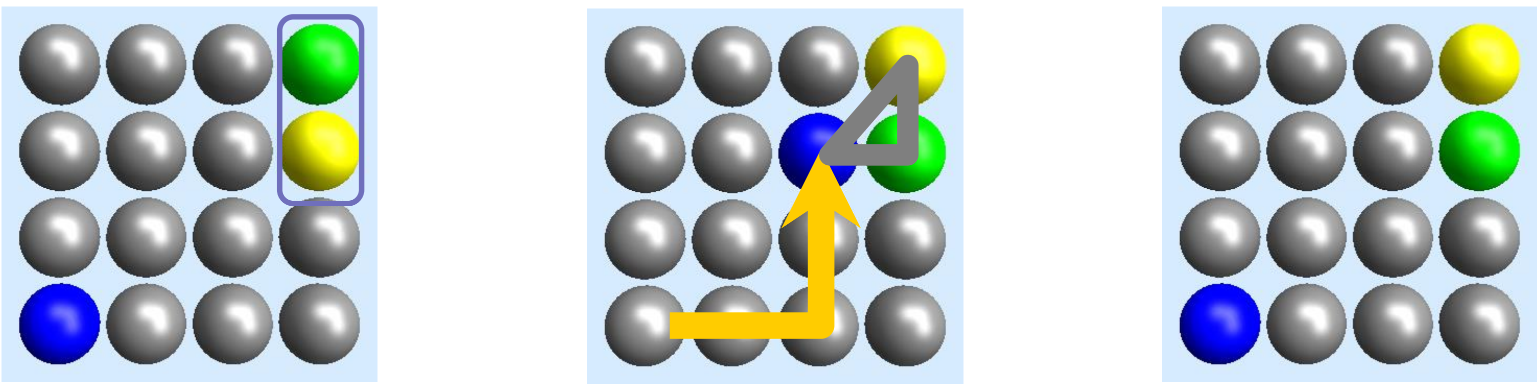

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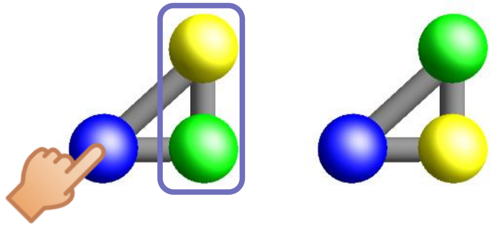

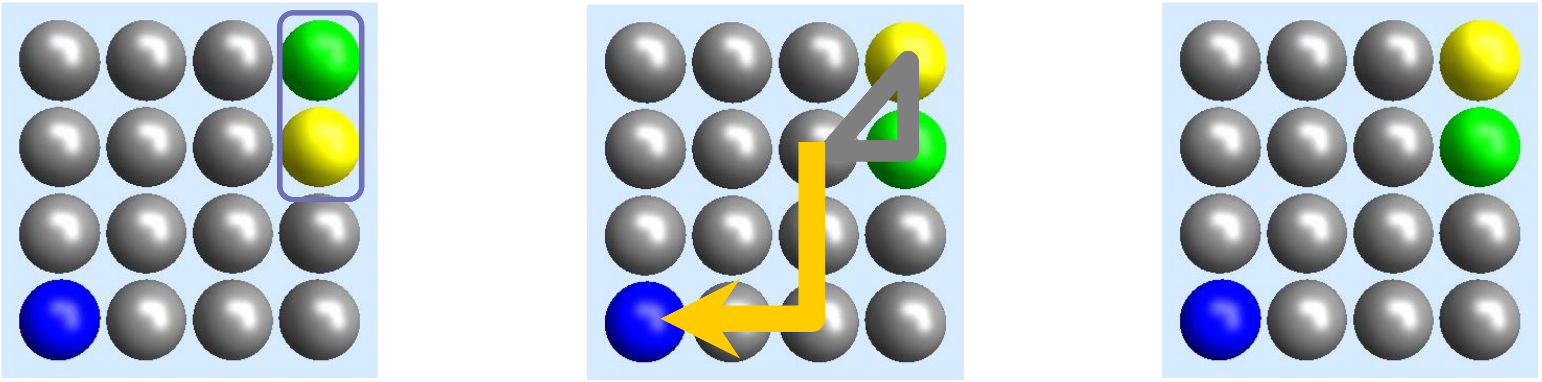

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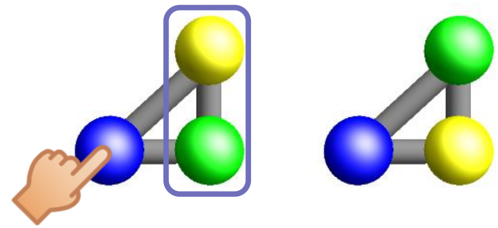
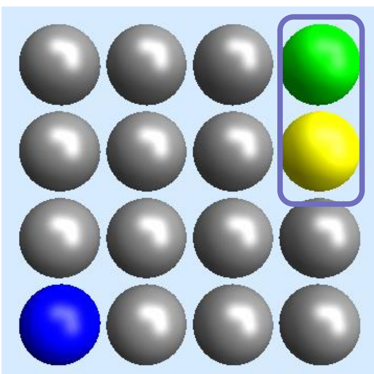
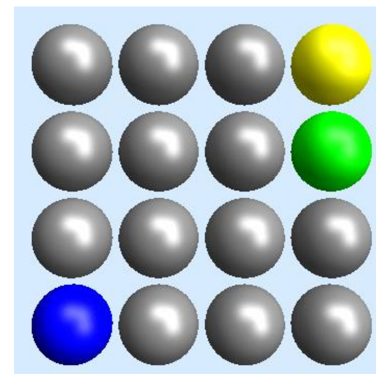




青の移動のみで
互換を構成できる！
灰色の配置はそのまま



■ PF定理が適用できる基底がある

$$|i,\boldsymbol{\alpha}\rangle = (-1)^i c^\dagger_{1,\alpha_1} \cdots c^\dagger_{i-1,\alpha_{i-1}} c^\dagger_{i+1,\alpha_{i+1}} \cdots c^\dagger_{|\Lambda|,\alpha_{|\Lambda|}} |\mathrm{vac}\rangle$$

A crash course in inequalities

Positive semidefinite operators

Appendix in H.Tasaki, *PTP.* **99**, 489 (1998) or his book

$\mathcal{H}$: finite-dimensional Hilbert space

A, *B*: Hermitian operators on $\mathcal{H}$

- **Definition 1.** We write $A \geq 0$ and say *A* is positive semidefinite (p.s.d.) if $\langle\psi|A|\psi\rangle \geq 0, \ \forall|\psi\rangle \in \mathcal{H}.$
- **Definition 2.** We write $A \geq B$ if $A - B \geq 0.$

Important lemmas

- **Lemma 1.** $A \geq 0$ iff all the eigenvalues of *A* are nonnegative.
- **Lemma 2.** Let C be an arbitrary matrix on $\mathcal{H}$. Then $C^\dagger C \geq 0.$
  Cor. A projection operator $P = P^\dagger$ is p.s.d.
- **Lemma 3.** If $A \geq 0$ and $B \geq 0$, we have $A + B \geq 0.$

Frustration-free systems

■ Anderson's bound (*Phys. Rev*. **83**, 1260 (1951).)

- Total Hamiltonian: $H = \sum_j h_j$
- Sub-Hamiltonian: h_j that satisfies $h_j \geq E_j^{(0)} \mathbf{1}$.
  ($E_j^{(0)}$: the lowest eigenvalue of h_j)

(The g.s. energy of *H*) =: $E_0 \geq \sum_j E_j^{(0)}$

Used to obtain a lower bound on the g.s. energy of AFM Heisenberg model

■ Frustration-free Hamiltonian

The case where the *equality* holds.

Definition. $H = \sum_j h_j$ is said to be *frustration-free* if there exists a state $|\psi\rangle$ such that $h_j|\psi\rangle = E_j^{(0)}|\psi\rangle$ for all *j*.

Ex.) *S*=1 Affleck-Kennedy-Lieb-Tasaki (AKLT), toric code

$$H = \sum_j h_j, \quad h_j = \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + \frac{1}{3}(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})^2$$

Flat-band ferro. is another example!

Hopping term

Diagonalization

Boils down to the diagonalization of T=($t_{x,y}$)

$$H_{\rm hop} = \sum_{\alpha=1}^{N} \sum_{x,y\in\Lambda} t_{x,y} c^\dagger_{x,\alpha} c_{y,\alpha}$$

- Eigen-operators

Let ***v*** be an eigenvector of T with eigenvalue ϵ.
Then, the operator

$$\psi^\dagger_\alpha = \sum_{x\in\Lambda} v_x c^\dagger_{x,\alpha} \quad \text{satisfies} \quad [H_{\rm hop}, \psi^\dagger_\alpha] = \epsilon \psi^\dagger_\alpha.$$

Acting with $\psi^\dagger_\alpha$ on an eigenstate of $H_{\rm hop}$ raises energy by ϵ.

- Eigenstates

$|{\rm vac}\rangle$ is an eigenstate of $H_{\rm hop}$ with energy 0.

General eigenstates take the form: $\psi^{\dagger(1)}_\alpha \psi^{\dagger(2)}_\beta \psi^{\dagger(3)}_\gamma \cdots |{\rm vac}\rangle$
where $\mathrm{T}\boldsymbol{v}^{(k)} = \epsilon^{(k)} \boldsymbol{v}^{(k)},\ \psi^{\dagger(k)}_\alpha = \sum_{x\in\Lambda} v^{(k)}_x c^\dagger_{x,\alpha}$

Interaction Term

■ Diagonalization

Already diagonal in the number basis!

$$H_{\mathrm{int}} = U \sum_{1 \le \alpha < \beta \le N} \sum_{x \in \Lambda} n_{x,\alpha} n_{x,\beta}$$

- Eigenstates

$c^\dagger_{x,\alpha} c^\dagger_{y,\beta} c^\dagger_{z,\gamma} \cdots |\mathrm{vac}\rangle$ is an eignstate of H_{int}.

For example, $c^\dagger_{x,1} c^\dagger_{x,2} c^\dagger_{y,3} c^\dagger_{z,1} c^\dagger_{z,3} |\mathrm{vac}\rangle$ has energy $2U$.

What about the full Hamiltonian?

- Hopping and interaction terms do not commute!

$$[H_{\mathrm{hop}}, H_{\mathrm{int}}] \neq 0$$

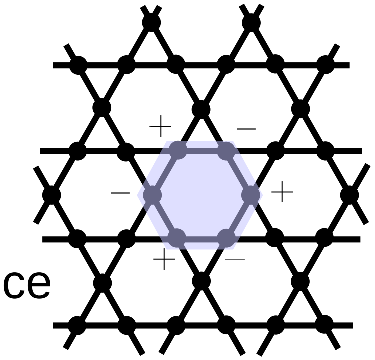
- Not even frustration-free in general…

But for a hopping term with a *flat band* (at the bottom), the full Hamiltonian becomes frustration-free!

What are flat bands?

- Single-particle eigenstates of H_{hop}

$$H_{\mathrm{hop}} = \sum_{\alpha=1}^{N} \sum_{x,y\in\Lambda} t_{x,y} c^\dagger_{x,\alpha} c_{y,\alpha}$$

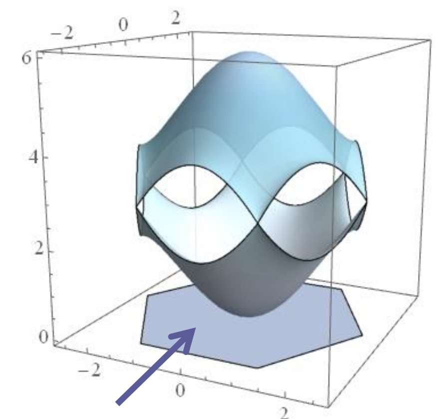


Kagome lattice

  - Energy bands

    In systems with translation symmetry, wave-num. $\boldsymbol{k}$ is a good quantum number.

$$H_{\mathrm{hop}}\psi^\dagger_\alpha(\boldsymbol{k})|\mathrm{vac}\rangle = \epsilon(\boldsymbol{k})\psi^\dagger_\alpha(\boldsymbol{k})|\mathrm{vac}\rangle$$



Band structure

  - Flat band

    Single-particle energy $\epsilon(\boldsymbol{k})$ is independent of $\boldsymbol{k}$.

- Various constructions
  - Line-graph construction: Mielke
  - Cell construction: Tasaki
  - Imbalance-type: Sutherland, …
  - Resonance-type: Katsura-Maruyama, Mizoguchi *et al*., …

解説記事:
桂, 丸山, "フラットバンドの構成法"
固体物理 **50**, 41 (2015) [ネットにあり]

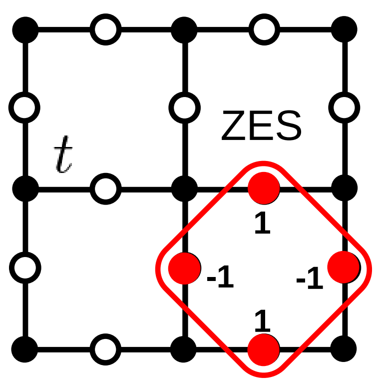
Index theorem & flat band

■ Sutherland's paper [*PRB* **34**, 5208 (1986)]

> Finally, as pointed out by Sriram Shastry, these results seem to be related to deep theorems of differential geometry, such as the Atiyah-Singer index theorem, although the exact connections are yet to be made.

■ Sublattice asymmetry

Lieb lattice



- Hopping matrix

$$\mathsf{T} = \begin{pmatrix} O & B \\ B^\dagger & O \end{pmatrix} \qquad B\text{: } N_\bullet \times N_\circ \text{ matrix}$$

- γ_5 matrix

$$\gamma_5 = \mathrm{diag}(\overbrace{-1, \cdots -1}^{N_\bullet}, \overbrace{+1, \cdots +1}^{N_\circ})$$

$$\{\gamma_5, \mathsf{T}\} = 0$$

- $\dim \mathrm{Ker}\,\mathsf{T} \geq N_\circ - N_\bullet$

Why frustration-free?

- Assume p.s.d. Hopping matrix $\mathsf{T} \geq 0$
- Kernel of *T* spanned by orthonormal $\boldsymbol{v}^{(j)}$ $(j=1,\cdots,D_0)$, $\mathsf{T}\boldsymbol{v}^{(j)}=0$
- Zero-energy eigen-operators $a^{\dagger}_{j,\alpha}=\sum_{x\in\Lambda} v^{(j)}_x c^{\dagger}_{x,\alpha}$ $\quad [H_{\mathrm{hop}}, a^{\dagger}_{j,\alpha}]=0$
- Interaction term is p.s.d. for *U* >0
- Many-body zero-energy state $|\Phi_{\mathrm{ferro},\alpha}\rangle = \left(\prod_{j=1}^{D_0} a^{\dagger}_{j,\alpha}\right)|\Phi_{\mathrm{vac}}\rangle$

  Because of the Pauli principle $(c^{\dagger}_{x,\alpha})^2=0$,

  $H_{\mathrm{hop}}|\Phi_{\mathrm{ferro},\alpha}\rangle = H_{\mathrm{int}}|\Phi_{\mathrm{ferro},\alpha}\rangle = 0$ Frustration-free!

Are they unique (up to trivial degeneracy)?

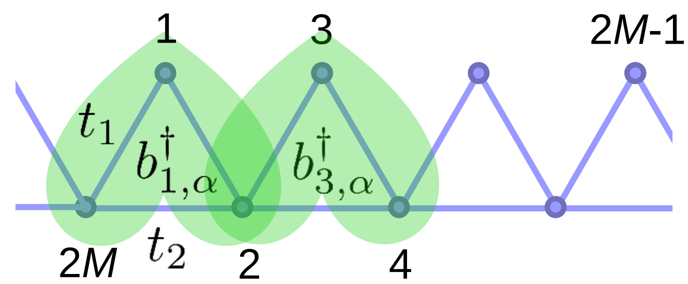
- In the SU(2) case, Mielke established a necessary and sufficient condition for the uniqueness [Mielke, Phys. Lett. A **174**, 443 (1993)]
- SU(*N*) への一般化: 田村さんの午後のトーク

Model on 1D Tasaki lattice

Lattice and hopping term

- Lattice: $\Lambda = \{1, 2, ..., 2M\}$

  $\mathcal{O} = \{1, 3, 5, ...\}, \ \mathcal{E} = \{2, 4, 6, ...\}$



$$t_1 = \nu t, \ t_2 = \nu^2 t,$$

$$t_{x,x} = t \text{ if } x \in \mathcal{O}, \ t_{x,x} = 2\nu^2 t \text{ if } x \in \mathcal{E}$$

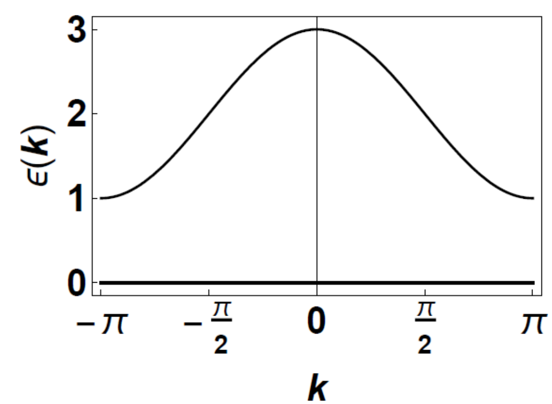
- Periodic boundary conditions:
  Identify site *j* with *j*+2*M*

- Hopping term (t >0)

$$H_{\text{hop}} = \sum_{\alpha=1}^{N} \sum_{x,y\in\Lambda} t_{x,y} c^\dagger_{x,\alpha} c_{y,\alpha} = t \sum_{\alpha=1}^{N} \sum_{x\in\mathcal{O}} b^\dagger_{x,\alpha} b_{x,\alpha}$$

$$b_{x,\alpha} := \nu c_{x-1,\alpha} + c_{x,\alpha} + \nu c_{x+1,\alpha}, \quad x \in \mathcal{O}$$

$$t = 1, \ \nu = 1/\sqrt{2}$$



Localized eigen-operators of H_{hop}

$$a_{x,\alpha} = -\nu c_{x-1,\alpha} + c_{x,\alpha} - \nu c_{x+1,\alpha}, \quad x \in \mathcal{E}$$

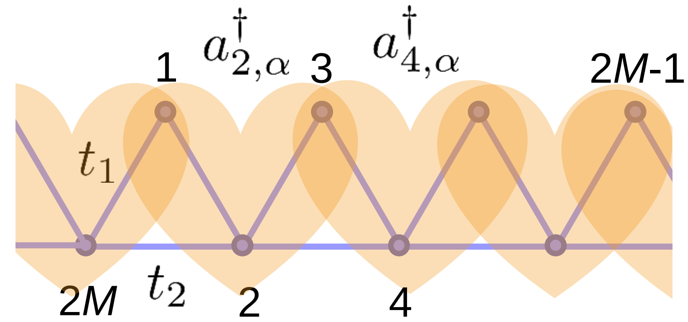
$$[H_{\text{hop}}, a^\dagger_{x,\alpha}] = 0 \ \ (\because \{a^\dagger_{x,\alpha}, b_{y,\beta}\} = 0)$$

The flat band is spanned by *a*-operators.

Model on 1D Tasaki lattice

■ Lattice and hopping term

- Lattice: $\Lambda = \{1, 2, \ldots, 2M\}$
  $\mathcal{O} = \{1, 3, 5, \ldots\},\ \mathcal{E} = \{2, 4, 6, \ldots\}$
- Periodic boundary conditions:
  Identify site *j* with *j*+2*M*



$t_1 = \nu t,\ t_2 = \nu^2 t,$

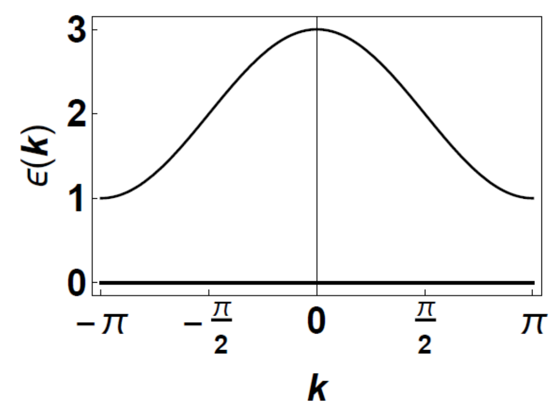
$t_{x,x} = t \text{ if } x \in \mathcal{O},\ t_{x,x} = 2\nu^2 t \text{ if } x \in \mathcal{E}$

- Hopping term (*t* >0)

$$H_{\mathrm{hop}} = \sum_{\alpha=1}^{N} \sum_{x,y\in\Lambda} t_{x,y} c^\dagger_{x,\alpha} c_{y,\alpha} = t \sum_{\alpha=1}^{N} \sum_{x\in\mathcal{O}} b^\dagger_{x,\alpha} b_{x,\alpha}$$

$$b_{x,\alpha} := \nu c_{x-1,\alpha} + c_{x,\alpha} + \nu c_{x+1,\alpha}, \quad x \in \mathcal{O}$$

$t = 1,\ \nu = 1/\sqrt{2}$



■ Localized eigen-operators of H_{hop}

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$$[H_{\mathrm{hop}}, a^\dagger_{x,\alpha}] = 0 \ \ (\because \{a^\dagger_{x,\alpha}, b_{y,\beta}\} = 0)$$

The flat band is spanned by *a*-operators.

Flat-band ferromagnetism

■ SU(*N*) Ferromagnetic (FM) states

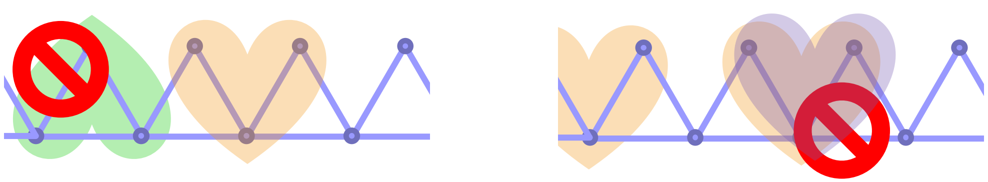
- Fix total fermion num.: $F_{\mathrm{tot}} = M$ The num. of unit cells
- Fully polarized states $|\Phi_{\mathrm{all},\alpha}\rangle := \left(\prod_{x\in\mathcal{E}} a^{\dagger}_{x,\alpha}\right)|\mathrm{vac}\rangle, \quad \alpha = 1, ..., N$

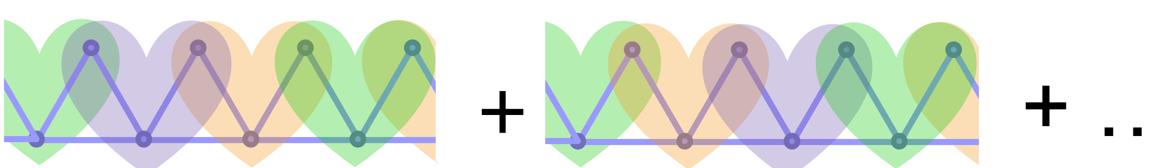
  are ground states (g.s.) of $H = H_{\mathrm{hop}} + H_{\mathrm{int}}$
  as they simultaneously minimize H_{hop} and H_{int}

  Frustration-free!
- Other FM g.s.: $(F^{N,1})^{F_N}\cdots(F^{2,1})^{F_2}|\Phi_{\mathrm{all},1}\rangle$
- Total num. of FM states: $d_{\mathrm{deg}} = \dfrac{(M+N-1)!}{M!(N-1)!}$

■ Uniqueness of FM g.s.

- Appearance of *b* and multiple occupancy of *a* are prohibited

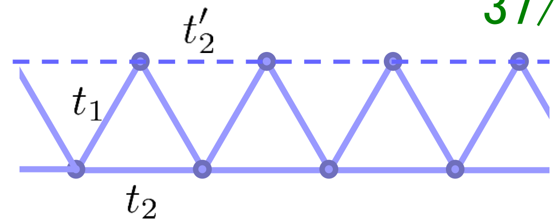




Must be symmetric under permutations of colors

Model with nearly flat band

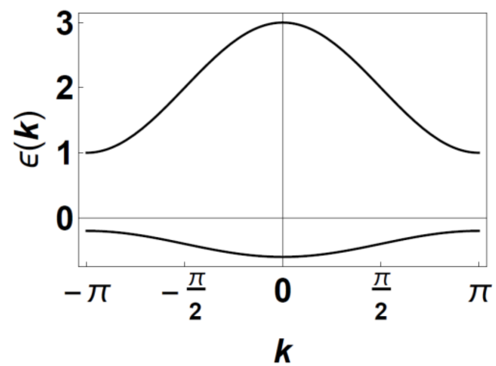
■ Lattice and hopping term



$$t_1 = \nu(t+s),\ t_2 = \nu^2 t,\ t_2' = -\nu^2 s$$

$$t_{x,x} = t - 2\nu^2 s \text{ if } x \in \mathcal{O}$$

$$t_{x,x} = -s + 2\nu^2 t \text{ if } x \in \mathcal{E}$$



- Hopping term (t >0, s >0)

$$H_{\text{hop}} = -\,s \sum_{\alpha=1}^{N} \sum_{x\in\mathcal{E}} a^{\dagger}_{x,\alpha} a_{x,\alpha} + t \sum_{\alpha=1}^{N} \sum_{x\in\mathcal{O}} b^{\dagger}_{x,\alpha} b_{x,\alpha}$$

- Total Hamiltonian $H = H_{\text{hop}} + H_{\text{int}}$

■ Theorem Tamura & Katsura, PRB **100** (2019)

Consider the Hubbard Hamiltonian H with the total fermion number $F_{\text{tot}}=M$. For sufficiently large t/s >0 and U/s >0, the ground states of H are SU(N) ferromagnetic and unique apart from trivial degeneracy due to the SU(N) symmetry.

- SU(N) generalization of Tasaki, *PRL* **75**, 4678 (1995)
- Higher-dim. generalization: Tamura & Kasura, *JSP* **182**, 16 (2021)

Outline

1. Introduction

2. 強磁性についての厳密な結果

3. 引力Hubbard模型についての厳密な結果

- マヨラナ鏡映とは？
- 主要な結果

4. Summary

Rigorous results for attractive Hubbard

	SU(2), U<0	SU(N), N>2, U<0
Method	Spin reflection positivity $c_{x,\uparrow} \leftrightarrow c_{x,\downarrow}$	Majorana reflection positivity $\gamma^{(1)}_{x,\alpha} \leftrightarrow \gamma^{(2)}_{x,\alpha}$
Ground-state degeneracy	Unique for N_e=even Lieb, PRL **62** (1989)	At most doubly degenerate in the whole Fock space
Rep. of g.s.	G.S. is SU(2) singlet Lieb, PRL **62** (1989)	G.S. is SU(N) singlet
Correlation function	$\langle \Phi_{\rm GS} \vert c^\dagger_{x,\uparrow} c^\dagger_{x,\downarrow} c_{y,\downarrow} c_{y,\uparrow} \vert \Phi_{\rm GS} \rangle > 0$ G-S. Tian, PRB **45** (1992)	$\langle \Phi_{\rm GS} \vert S_{x,y} \vert \Phi_{\rm GS} \rangle > 0$
Long-range order (LRO) for $\vert A\vert$-$\vert B\vert$ = O($\vert\Lambda\vert$)	Off-diagonal LRO Shen & Qiu, PRL **71** (1993) Charge-density wave G-S. Tian, PLA **192** (1994)	Charge-density wave Yoshida & Katsura, PRL **126**, 100201 (2021)

Model

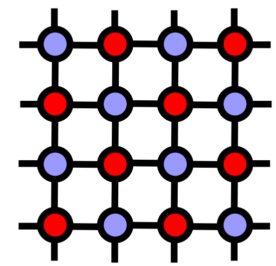
■ Hamiltonian

$$n_x = \sum_{\alpha=1}^{N} n_{x,\alpha}$$

$$H = \sum_{\alpha=1}^{N} \sum_{x,y\in\Lambda} t_{x,y}(c^\dagger_{x,\alpha} c_{y,\alpha} + c^\dagger_{y,\alpha} c_{x,\alpha}) + \sum_{x\in\Lambda} U_x \left(n_x - \frac{N}{2} \right)^2$$

Assumptions:

1. $N \geq 3$
2. Lattice is bipartite ($\Lambda = A \cup B$) and connected.
   Examples: square, cubic, Lieb, …
3. Hopping matrix $\mathsf{T} = (t_{x,y})_{x,y\in\Lambda}$ is real symmetric
   $t_{x,y} = 0$ if *x* and *y* are on the same sublattice
4. $U_x < 0$ for all $x \in \Lambda$



■ SU(*N*) symmetry (reminder) and singlet

- Hamiltonian commutes with $F^{\alpha,\beta} := \sum_{x\in\Lambda} c^\dagger_{x,\alpha} c_{x,\beta}$
- SU(*N*) singlet: a state invariant under SU(*N*) rotation

$$F^{\alpha,\beta}|\Phi_{\rm sing}\rangle = 0 \ \forall\alpha \neq \beta, \quad F^{1,1}|\Phi_{\rm sing}\rangle = \cdots = F^{N,N}|\Phi_{\rm sing}\rangle$$

What is Majorana reflection?

Majorana fermions

$$\gamma^{(1)}_{x,\alpha} := c_{x,\alpha} + c^{\dagger}_{x,\alpha}, \quad \gamma^{(2)}_{x,\alpha} := -\mathrm{i}(c_{x,\alpha} - c^{\dagger}_{x,\alpha}) \quad \text{for } x \in A$$

$$\gamma^{(1)}_{x,\alpha} := -\mathrm{i}(c_{x,\alpha} - c^{\dagger}_{x,\alpha}), \quad \gamma^{(2)}_{x,\alpha} := c_{x,\alpha} + c^{\dagger}_{x,\alpha} \quad \text{for } x \in B$$

- They obey $(\gamma^{(j)}_{x,\alpha})^{\dagger} = \gamma^{(j)}_{x,\alpha}$ and $\{\gamma^{(j)}_{x,\alpha}, \gamma^{(k)}_{y,\beta}\} = 2\delta_{j,k}\delta_{x,y}\delta_{\alpha,\beta}$

Hamiltonian in terms of Majoranas

$$H_{\mathrm{hop}} = \sum_{\alpha=1}^{N} \sum_{x\in A, y\in B} t_{x,y} \left(\frac{\mathrm{i}}{2}\gamma^{(1)}_{x,\alpha}\gamma^{(1)}_{y,\alpha} - \frac{\mathrm{i}}{2}\gamma^{(2)}_{x,\alpha}\gamma^{(2)}_{y,\alpha} \right)$$

$$H_{\mathrm{int}} = \sum_{\alpha,\beta} \sum_{x\in\Lambda} U_x \left(\frac{\mathrm{i}}{2}\gamma^{(1)}_{x,\alpha}\gamma^{(1)}_{x,\beta} \right) \left(-\frac{\mathrm{i}}{2}\gamma^{(2)}_{x,\alpha}\gamma^{(2)}_{x,\beta} \right)$$

They are invariant under *θ*

Majorana reflection

QMC literature: Wei *et al*., *PRL* **116** (2016)

- Anti-linear map:

$$\theta(\gamma^{(1)}_{x,\alpha}) = \gamma^{(2)}_{x,\alpha}, \quad \theta(\gamma^{(2)}_{x,\alpha}) = \gamma^{(1)}_{x,\alpha}, \quad \theta(\mathrm{i}) = -\mathrm{i}$$

Main results

■ Theorem 1 (singlet g.s.)

- $|A| \neq |B|$ → Exactly two ground states. They are SU(N) singlet.
  Their fermion num. are $N|A|$ and $N|B|$, respectively.

- $|A| = |B|$ → At most two ground states, each of which is
  SU(N) singlet with $F_{\mathrm{tot}} = N|A|$ (= $N|B|$).

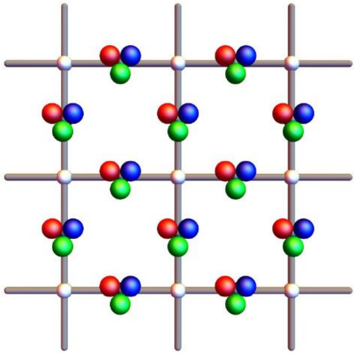
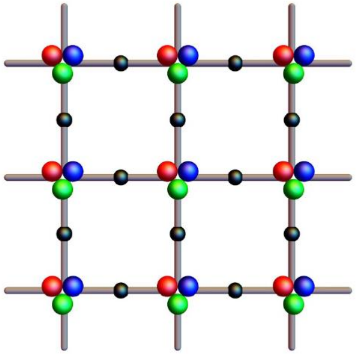
■ Theorem 2 (correlation function)

- Consider the operator $S_{x,y} = (-1)^x(-1)^y \left(n_x - \frac{N}{2}\right)\left(n_y - \frac{N}{2}\right)$,
  where $(-1)^x = 1$ for $x \in A$ and $(-1)^x = -1$ for $x \in B$.

- For any g.s. $|\Phi_{\mathrm{GS}}\rangle$ and for any $x, y \in \Lambda$, $\langle\Phi_{\mathrm{GS}}|S_{x,y}|\Phi_{\mathrm{GS}}\rangle > 0$.

■ Perturbative picture

- Model with $|U| \gg |t_{x,y}|$ exhibits checkerboard patterns in g.s.
- Ex.) SU(3) model on Lieb lattice

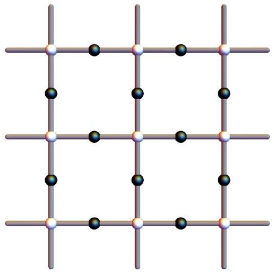



Main results (cont'd)

■ Theorem 3 (charge density wave)

- $|A| - |B| = a|\Lambda|$ $(-1 < a < 1)$
- Define order parameter $S = \sum_{x\in\Lambda}(-1)^x\left(n_x - \frac{N}{2}\right)$
- Then for any g.s. $|\Phi_{\mathrm{GS}}\rangle$,

  we have $\langle\Phi_{\mathrm{GS}}|S^2|\Phi_{\mathrm{GS}}\rangle > \left(\frac{aN|\Lambda|}{2}\right)^2$



What is Majorana reflection positivity?

- Eigen-operator of *H*: $HO = OH = EO$
- Expansion of *O*: $O(W) = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{C}_{\mathrm{even}}} W_{\boldsymbol{\alpha},\boldsymbol{\beta}}\Gamma^{(1)}_{\boldsymbol{\alpha}}\Gamma^{(2)}_{\boldsymbol{\beta}}$

$$\Gamma^{(1)}_{\boldsymbol{\alpha}} = \mathrm{i}^{\lfloor \ell(\boldsymbol{\alpha})\rfloor}\gamma^{(1)}_{x_1,\alpha_1}\gamma^{(1)}_{x_1,\alpha_2}\cdots,$$

$$\Gamma^{(2)}_{\boldsymbol{\alpha}} = (-\mathrm{i})^{\lfloor \ell(\boldsymbol{\alpha})\rfloor}\gamma^{(2)}_{x_1,\alpha_1}\gamma^{(2)}_{x_1,\alpha_2}\cdots$$

- Define $|W| := \sqrt{W^\dagger W}$
- Can show $E(|W|) \le E(W)$.

概要:

本講演では、強磁性・スピン鏡映正値性・ηペアリング対称性などのSU(2)ハバード模型における既知の厳密な結果について概観した後に、それらの結果のSU(N)ハバード模型における拡張を紹介する。
また時間が許せば、散逸のあるハバード模型や量子多体傷跡状態など、…

η-paring states

- Exact eigenstates of SU(2) Hubbard model
  - Hamiltonian $H = \sum_{\sigma=\uparrow,\downarrow} \sum_{x,y\in\Lambda} t_{x,y} c^\dagger_{x,\sigma} c_{y,\sigma} + U \sum_{x\in\Lambda} n_{x,\uparrow} n_{x,\downarrow}$
  - Assume bipartite Λ
  - *η* operator $\eta^\dagger := \sum_{x\in\Lambda} (-1)^x c^\dagger_{x,\uparrow} c^\dagger_{x,\downarrow}$ C.N. Yang, *PRL* **63**, 2144 (1989)
  - $|\psi_k\rangle = (\eta^\dagger)^k |\mathrm{vac}\rangle$ is an eigenstate of *H* with eigenvalue *Uk*
  - $|\psi_k\rangle \quad (k = 1, 2, ...)$ are not ground states
  - They exhibit off-diagonal long-range order (ODLRO)
- SU(*N*) extensions
  - *η*-pairing states in SU(*N*) Hubbard model
    Nakagawa, Katsura & Ueda, arXiv:2205.07235
  - η-clustering states in 1d extended SU(*N*) Hubbard model
    Yoshida & Katsura, *PRB* **105**, 024520 (2022)

Summary

- 長岡強磁性のSU(*N*)への拡張
- 平坦バンド強磁性のSU(*N*)への拡張
- ほとんど平坦なバンドの場合についても拡張
- 引力SU(*N*) Hubbard模型の基底状態の諸性質
- ηペアリング状態のSU(*N*)への拡張