Exact results in strongly correlated electrons

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This article is devoted to discuss two exact arguments in strongly-correlated electron systems: one is the method of reflection positivity in spin space and the other is the Perron-Frobenius theorem in matrix theory. For several specific systems, we can show that the ground state is unique and we can predict the total spin of the ground state.

Contents

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1. Introduction

Strongly correlated electron systems have been studied considerably in recent years. Heavy fermions[1,2,3] and oxide superconductors[4] provide attractive problems for researchers of solid state physics. The fundamental models to describe strongly-correlated electrons are given by the Hubbard model, the Anderson lattice and the Kondo lattice Hamiltonian.

The Hubbard model has a long history in describing the magnetism of materials since early works by Hubbard, Gutzwiller and Kanamori.[5,6,7] The Hubbard model has attracted much attention recently, stimulated by studies of high-T_c superconductors.[8,9,10] Thus the importance of the Hubbard model of itinerant electrons is increasingly being appreciated. One-dimensional Hubbard model is now understood in a very elegant way by means of the Bethe ansatz [11,12,13] and conformal field theory.[14,15,16] The solutions revealed that the weak-coupling bosonization theory[17,18] can well describe the ground state of the 1D Hubbard model, which established a novel concept of the Luttinger liquid.[19] In spite of the success for the one-dimensional correlated models such as the Hubbard model and the t-J model, correlated electrons in two- or three-dimensional space are still far from a complete understanding. In the study of the Hubbard model, main topics are likely the following:

(H1) Metal-insulator transition: Metal or Insulator?
(H2) Magnetism: Ferromagnetism or Antiferromagnetism?
(H3) Possibility of a superconductivity.
(H4) Fermi liquid or non-Fermi liquid.
(H5) Quantum Critical Phenomena.

The topic (H1) concerns the Mott transition due to large Coulomb repulsion.[20] In this article, of central importance is given by (H2): the magnetism of the Hubbard model. The magnetism is intrinsically given by quantum many-body effects which mainly arises from the strong Coulomb interactions.[21] Quantum effects prevent us from easy understanding of antiferromagnetism or ferromagnetism of itinerant electrons.[22] Recently the non-Fermi liquid behaviors associated with quantum critical phenomema have attracted much attention. [23,24,25,26] Thus exact results are important as bench marks although they are limited to special cases.

The Kondo lattice Hamiltonian or the periodic Anderson model (or Anderson lattice Hamiltonian) are established as models to describe heavy fermions that contain rare-earth or actinide ions and show very characteristic behaviors. In particular, they have large electron densities of states which are accompanied by a linear specific heat and an almost temperature independent spin susceptibility. They behave like Fermi liquids with very heavy mass which can become as large as several hundred or a thousand times the free electron mass.[1,2,3] These systems can be described by

the conduction electrons and the localized f electrons which interact through a hybridization interaction or an exchange type of interaction. The following are likely to be questions concerning the Kondo lattice or the Anderson lattice Hamiltonian:

(K1) Fermi liquid state with heavy mass.
(K2) Interplay between the Kondo effect[27,28] and the RKKY interactions.[29,30,31]
(K3) Magnetism: Ferromagnetism or Antiferromagnetism?
(K4) Anisotropic superconductivity.[32]
(K5) Metal-Insulator transition: Kondo insulators.
(K6) Antiferromagnetism and superconductivity: Coexistence.
(K7) Quantum critical phenomena: Non-Fermi liquid.[25,26]

Similar issues are addressed for the Kondo systems compared to the Hubbard model except (K1) and (K2). If we remember the long debate concerning the Kondo problem, obviously they are not easy task to find solutions. As for the problem (K5), SmB_6 and YbB_{12} provide us examples of Kondo insulators,[33,34,35,36] which can be modeled as the Anderson lattice in which we have one electron at each site, corresponding to the quarter-filled case. We also comment that there are theories which insist that Kondo insulators may be described by the half-filled Anderson lattice model.[37,38] The Kondo matrials such as CeNiSn[39,40,41] are also known as Kondo insulators or low-carrier Kondo systems. It should be considered that several types of Kondo insulators show completely different behaviors. As for the compound Yb_4As_3, a mechanism of the metal-insulator transition due to a concept of 'self-doping' was recently proposed.[42,43] Recently, impurities embedded in correlated electrons are becoming a hot subject.[44,45,46,47]

In this paper, let us investigate two methods which sometimes provide us exact information: they are the reflection positivity in the spin space and the Perron-Frobenius theorem. First, we discuss the method of the reflection positivity in the spin space. This method was first applied to the negative-U Hubbard model with an even number of electrons and the positive-U Hubbard model at half filling.[48] We start from writing a wave function in a matrix form.[49] If the matrix can be shown to be positive semidefinite, a uniqueness of the ground state is proved. This method is called the reflection positivity in the spin space (or the spin-reflection positivity) in analogy with the reflection positivity in field theory.[50] We apply this method to the Heisenberg model, the Kondo lattice and the Kondo-Hubbard model for the half-filled conduction band. The spin-correlation functions such as $\langle S_i^+ S_j^- \rangle$ are proved to have definite signs. The spin-reflection positivity is clearly related to the antiferromagnetic correlations in the Heisenberg model and the positive-U Hubbard model at half filling. In a proof of the spin-reflection positivity, we make a partial electron-hole transformation where the spin operators are transformed into the η-spin (or pseudo spin) operators. Thus we shall add a section to discuss some properties of η-operators.

Second, let us discuss the Perron-Frobenius theorem applied to many-electron

systems. The Chapter **3** is devoted to present the Perron-Frobenius theorem and its proof. This Chapter can be skipped if readers are familiar with the Perron-Frobenius theorem. In the Chapter **4**, we discuss several examples of correlated electron systems for which the Perron-Frobenius theorem is applicable. A first one is the Heisenberg model which was considered by Lieb and Mattis more than thirty years ago. Secondly, the double exchange interaction is discussed in the light of the Perron-Frobenius theorem, which may be important for the ferromagnetism of solid. The double exchange has a long history and its relevance may be realized in the Kondo systems. In several limits of parameters included in the Kondo lattice or the Anderson lattice Hamiltonians, we can expect the ferromagnetism due to the double exchange interaction. Thirdly, the Nagaoka ferromagnetism is discussed from the viewpoint of the Perron-Frobenius theorem. The last Chapter is devoted to some remarks.

In the remaining part of Introduction, we shall introduce the Hubbard model, the Anderson model (lattice) and the Kondo model (lattice) in order to indicate notations in this paper. This part can be skipped if readers are acquainted with them. Let us start with the Hubbard model written as[5]

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{\downarrow}, \tag{1}$$

where $c^{\dagger}_{i\sigma}$ ($c_{i\sigma}$) denote the creation (annihilation) operators of electrons and $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ are number operators. t_{ij} and U are parameters which control the electron states and the other important parameter is the dimensionality of space. The U-term represents the Coulomb interaction which works when the two electrons occupy the same site. We denote the number of lattice sites and electrons as N and N_e, respectively. Although the Hamiltonian (1) is quite simple, its understanding is extraordinary difficult and it may form one of the high mountains in theoretical physics. In most cases we assume that t_{ij} are non-zero between nearest-neighbor sites. In the non-interacting limit $U = 0$, the Hamiltonian is easily diagonalized by introducing the Fourier transform of $c_{i\sigma}$. The ground state is obtained by filling the energy levels up to the Fermi energy. In the other limit $t_{ij} = 0$, each site is occupied by the up or down-spin electron, or is empty. This state is clearly insulating. The non-zero t_{ij} induce the movement of electrons, which leads to the metallic state if $N_e \neq N$. At half filling $N_e = N$, the ground state is considered to be insulating if U is large enough. This insulating state is described by the Heisenberg model given by

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{2}$$

In connection with the Hubbard model, J is given as $J = 4t^2/U$.[51] For the nearest-neighbor transfers $-t = t_{ij}$, the effective Hamiltonian for $N_e \neq N$ is given by

$$H = -t \sum_{\langle ij \rangle \sigma} a^{\dagger}_{i\sigma} a_{j\sigma} - \frac{t^2}{U} \sum_{j\mu\mu'} [a^{\dagger}_{j+\mu\uparrow} a^{\dagger}_{j\downarrow} a_{j\downarrow} a_{j+\mu'\uparrow} + a^{\dagger}_{j\uparrow} a^{\dagger}_{j+\mu\downarrow} a_{j+\mu'\downarrow} a_{j\uparrow}$$

$$+ \quad a^\dagger_{j+\mu\uparrow}a^\dagger_{j\downarrow}a_{j+\mu'\downarrow}a_{j\uparrow} + a^\dagger_{j\uparrow}a^\dagger_{j+\mu\downarrow}a_{j\downarrow}a_{j+\mu'\uparrow}], \tag{3}$$

where we have written $a_{i\sigma} = c_{i\sigma}(1 - n_{i,-\sigma})$ and $j + \mu$ and $j + \mu'$ indicate the nearest-neighbor sites. The second term involves three-site terms when $\mu \neq \mu'$.

The second fundamental models are the Anderson model[52] and its extension to the periodic case. The periodic Anderson model (or Anderson lattice Hamiltonian) is given by[53]

$$\begin{aligned} H &= \sum_{\langle ij\rangle\sigma} t_{ij}c^\dagger_{i\sigma}c_{j\sigma} + \epsilon_f \sum_{i\sigma} f^\dagger_{i\sigma}f_{i\sigma} \\ &+ V\sum_{i\sigma}(c^\dagger_{i\sigma}f_{i\sigma} + f^\dagger_{i\sigma}c_{i\sigma}) + U_f \sum_i n_{fi\uparrow}n_{fi\downarrow}, \end{aligned} \tag{4}$$

where $f^\dagger_{i\sigma}$ ($f_{i\sigma}$) are creation (annihilation) operators of the localized electron (f electrons) and we write $n_{fi\sigma} = f^\dagger_{i\sigma}f_{i\sigma}$. The last term shows the Coulomb interaction between the localized electrons If we introduce the wave number $\mathbf{k}$ for $c_{i\sigma}$:

$$c_{k\sigma} = \frac{1}{N^{1/2}}\sum_j e^{-ik\cdot R_j}c_{j\sigma}, \tag{5}$$

the Hamiltonian is written as

$$\begin{aligned} H &= \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma}c_{\mathbf{k}\sigma} + \epsilon_f \sum_{i\sigma} f^\dagger_{i\sigma}f_{i\sigma} \\ &+ \frac{1}{N^{1/2}}\sum_{jk\sigma}(V_k e^{-ik\cdot R_j}c^\dagger_{k\sigma}f_{j\sigma} + h.c.) + U_f \sum_i n_{fi\uparrow}n_{fi\downarrow}. \end{aligned} \tag{6}$$

The hybridization parameter V is generalized to include the $\mathbf{k}$-dependence. In the non-interacting case where $U_f = 0$, we have the upper and lower bands with the dispersions given by

$$E^\pm_k = \frac{\epsilon_k + \epsilon_f}{2} \pm [(\frac{\epsilon_k - \epsilon_f}{2})^2 + |V_k|^2]^{1/2}. \tag{7}$$

In the Kondo limit where the level of f electrons is located far below the Fermi level and U_f is large compared to t and V, the effective Hamiltonian is given by the Kondo lattice model

$$H = \sum_{ij\sigma} t_{ij}c^\dagger_{i\sigma}c_{j\sigma} + J\sum_i \sigma_i \cdot \mathbf{S}_i, \tag{8}$$

where σ_i and $\mathbf{S}_i$ denote the spin operators of the conduction electrons and localized electrons, respectively. σ^a_i ($a = x, y$ and z) is written as $\sigma^a_i = \sum_{\sigma\sigma'} c^\dagger_{i\sigma}\sigma^a_{\sigma\sigma'}c_{i\sigma'}$ where $\sigma^a_{\sigma\sigma'}$ are Pauli matrices. According to the Schrieffer-Wolff formula,[54] the exchange interaction is expressed as

$$J = V^2(\frac{1}{\epsilon_f + U} - \frac{1}{\epsilon_f}). \tag{9}$$

The Anderson lattice and the Kondo lattice are more hard to clarify their physics than the Hubbard model because of the two-band nature and may include fruitful physical phases. The above three models are fundamental in the solid state physics.

2. Reflection positivity in the spin space

2.1. *Basic method*

The purpose of the method of reflection positivity is to derive an inequality for the ground state energy based on the Schwarz inequality. In order to apply this method, we have to specify the lattice Λ and basis states on it. The number of the sites is denoted by $|\Lambda|$ and we assume that the number of lattice sites $|\Lambda|$ is finite. In this paper, let us consider the Hamiltonians which conserve $\mathbf{S}^2$ and S^z. The spin operators are the quadratic operators

$$S^+ = (S^-)^\dagger = \sum_{i\in\Lambda} c^\dagger_{i\uparrow} c_{i\downarrow}, \quad S^z = \frac{1}{2}\sum_{i\in\Lambda}(n_{i\uparrow} - n_{i\downarrow}), \tag{10}$$

and $\mathbf{S}^2 = (1/2)(S^+S^- + S^-S^+) + (S^z)^2$, with eigenvalues $S(S+1)$. We work in the subspace $S^z = 0$ for an even number of electrons. There are two kind of electrons with spin up and spin down. We denote a set of basis states as $X^\sigma \equiv \{\psi^\sigma_\alpha\}_{\alpha\in I}$ which is an orthonomal basis set composed solely of spin-σ electrons. (I denotes a set of indices.) The total bases are written as a superposition of the up and down basis states $\{\psi_{\alpha\beta} \equiv \psi^\uparrow_\alpha \otimes \psi^\downarrow_\beta\}$. Then a wave function is written as a linear combination of $\psi_{\alpha\beta}$: [49]

$$\psi = \sum_{\alpha\beta} C_{\alpha\beta}\psi^\uparrow_\alpha \otimes \psi^\downarrow_\beta. \tag{11}$$

The wave function ψ is represented by a coefficient matrix $C = (C_{\alpha\beta})$, which indicates that ψ can be interpreted as a map $C : X^\downarrow \to X^\uparrow$. We denote ψ as $\psi(C)$. $X^\uparrow$ and $X^\downarrow$ are vector spaces with the same finite dimension. Let us denote operators acting on the vector space X^σ as $\hat{O}^\sigma$, which are assumed to be products of an even number of operators such as $\hat{O}^\sigma = c^\dagger_{i\sigma}c_{j\sigma}$. It is easy to calculate an operation $\hat{O}^\sigma$ to ψ,

$$\begin{aligned}
\hat{O}^\uparrow\psi &= \sum_{\alpha\beta} C_{\alpha\beta}\hat{O}^\uparrow\psi_{\alpha\beta} = \sum_{\alpha\beta}\sum_{\alpha'\beta'} C_{\alpha\beta}|\psi_{\alpha'\beta'}\rangle\langle\psi_{\alpha'\beta'}|\hat{O}^\uparrow|\psi_{\alpha\beta}\rangle \\
&= \sum_{\alpha\beta}\sum_{\alpha'\beta'} C_{\alpha\beta}\psi_{\alpha'\beta'}\delta_{\beta\beta'}\langle\psi^\uparrow_{\alpha'}|\hat{O}^\uparrow|\psi^\uparrow_\alpha\rangle \\
&= \sum_{\alpha\beta\alpha'} (O^\uparrow)_{\alpha'\alpha} C_{\alpha\beta}\psi_{\alpha'\beta} \\
&= \sum_{\alpha\beta} (O^\uparrow C)_{\alpha\beta}\psi_{\alpha\beta},
\end{aligned} \tag{12}$$

where $(O^\uparrow)_{\alpha'\alpha} = \langle\psi^\uparrow_{\alpha'}|\hat{O}^\uparrow|\psi^\uparrow_\alpha\rangle$ are matrix elements of $\hat{O}^\uparrow$. $\hat{O}^\uparrow\psi$ is realized by a multiplication of matrices $O^\uparrow C$. Similarly, one can obtain

$$\hat{O}^\downarrow\psi = \sum_{\alpha\beta} C_{\alpha\beta}\hat{O}^\downarrow\psi_{\alpha\beta}$$

$$= \sum_{\alpha\beta\beta'} C_{\alpha\beta}(O^{\downarrow t})_{\beta\beta'}\psi_{\alpha\beta'}$$
$$= \sum_{\alpha\beta}(CO^{\downarrow t})_{\alpha\beta}\psi_{\alpha\beta}, \tag{13}$$

where $O^{\downarrow t}$ is the transposed matrix of $O^{\downarrow}$. An application of $\hat{O}^{\downarrow}$ to ψ reads $CO^{\downarrow t}$ in terms of coefficient matrix. It is easy to see that

$$\hat{O}^{\uparrow}\hat{O}^{\downarrow}\psi = \sum_{\alpha\beta}\sum_{\alpha'\beta'}(O^{\uparrow})_{\alpha'\alpha}C_{\alpha\beta}(O^{\downarrow t})_{\beta\beta'}\psi_{\alpha'\beta'}$$
$$= \sum_{\alpha\beta}(O^{\uparrow}CO^{\downarrow t})_{\alpha\beta}\psi_{\alpha\beta}. \tag{14}$$

In the following, we assume that the basis states are real so that matrices O^{σ} are real, which is always possible without loss of generality. Thus we write $O^{\sigma\dagger} = O^{\sigma t}$ in this paper. Now it is straightforward to write down the Schrödinger equations and the energy expectation values. Let us suppose that the Hamiltonian is given as

$$H = K^{\uparrow} + K^{\downarrow} + g\sum_a V_a^{\uparrow}V_a^{\downarrow}, \tag{15}$$

where K^{σ} and V_a^{σ} are operators for spin σ. The third term shows interactions between electrons and g is a coupling constant. We can choose the basis states so that K^{σ} and V_a^{σ} are real symmetric. We use the same notations to show matrices of K^{σ} and V_a^{σ}. The Schrödinger equation $H\psi = E\psi$ is written as

$$K^{\uparrow}C + CK^{\downarrow\dagger} + g\sum_a V_a^{\uparrow}CV_a^{\downarrow\dagger} = EC. \tag{16}$$

A hermitian conjugate of this equation reads

$$K^{\downarrow}C^{\dagger} + C^{\dagger}K^{\uparrow\dagger} + g\sum_a V_a^{\downarrow}C^{\dagger}V_a^{\uparrow\dagger} = EC^{\dagger}. \tag{17}$$

Hence, if we have the up-down symmetry of spin for basis states, C and $C^{\dagger}$ satisfy the same Schrödinger equation. Thus $C + C^{\dagger}$ and $C - C^{\dagger}$ are also solutions of the Schrödinger equation, and therefore we can assume that C is hermitian from the beginning. Note that two conditions (1) K^{σ} and V_a^{σ} are real and (2) $K^{\sigma} = K^{-\sigma}$, $V^{\sigma} = V^{-\sigma}$ (up-down symmetry) are needed to obtain the hermitian matrix C. Now, by applying $C^{\dagger}$ and taking Trace in eq.(16), the energy eigenvalue is easily calculated as

$$E(C) = Tr(C^{\dagger}K^{\uparrow}C + CK^{\downarrow}C^{\dagger}) + g\sum_a TrC^{\dagger}V_a^{\uparrow}CV_a^{\downarrow\dagger}, \tag{18}$$

with the normalization $\langle\psi|\psi\rangle = TrC^{\dagger}C = 1$. For $g < 0$, we can apply the Schwarz inequality:

$$TrC^{\dagger}V_aCV_a^{\dagger} \leq TrPV_aPV_a^{\dagger}, \tag{19}$$

where $V_a = V_a^{\uparrow} = V_a^{\downarrow}$ and P is the positive semidefinite matrix given as $P = (C^{\dagger}C)^{1/2}$. This inequality is easily proved as follows. Since C is hermitian, C can be diagonalized by a unitary matrix U:

$$C = U^{\dagger} \begin{bmatrix} \epsilon_1 & & & \\ & \epsilon_2 & & \\ & & . & \\ & & & . \end{bmatrix} U, \tag{20}$$

with real eigenvalues ϵ_α. An eigenvector which belongs to the eigenvalue ϵ_α is given by $|\alpha\rangle = U^{\dagger}(0, \cdots, 0, 1^{(\alpha)}, 0, \cdots, 0)^t$ which satisfies $C|\alpha\rangle = \epsilon_\alpha|\alpha\rangle$. Then,

$$\begin{aligned} TrC^{\dagger}VCV^{\dagger} &= \sum_{\alpha\beta}\langle\alpha|C^{\dagger}VC|\beta\rangle\langle\beta|V^{\dagger}|\alpha\rangle \\ &= \sum_{\alpha\beta}\epsilon_\alpha\epsilon_\beta\langle\alpha|V|\beta\rangle\langle\beta|V^{\dagger}|\alpha\rangle \\ &= \sum_{\alpha\beta}\epsilon_\alpha\epsilon_\beta|\langle\alpha|V|\beta\rangle|^2 \\ &\leq \sum_{\alpha\beta}|\epsilon_\alpha||\epsilon_\beta||\langle\alpha|V|\beta\rangle|^2 = TrPVPV^{\dagger}, \end{aligned} \tag{21}$$

where P is defined by

$$P = U^{\dagger} \begin{bmatrix} |\epsilon_1| & & & \\ & |\epsilon_2| & & \\ & & . & \\ & & & . \end{bmatrix} U. \tag{22}$$

P has $|\epsilon_\alpha|$ as eigenvalues and satisfies $P|\alpha\rangle = |\epsilon_\alpha||\alpha\rangle$. For negative values of g, we obtain an inequality

$$E(C) \geq E(P). \tag{23}$$

Therefore, if we assume that $\psi = \sum_{\alpha\beta} C_{\alpha\beta}\psi_{\alpha\beta}$ is the ground-state wave function, the following equality is followed:

$$E(C) = E(P). \tag{24}$$

This equation imposes strong constraints on the ground state, which enables us to show that the ground state is unique under some conditions. Apparently, $C = P$ is a solution of $E(C) = E(P)$. Hence there is a state which satisfies $C = P$ among the ground states.

In order to prove a uniqueness of the ground state, we should show that $C = P$ (or $C = -P$) is a unique solution of the equation $E(C) = E(P)$ because we easily reach a contradiction if we assume that there are two ground states.[48] For this purpose, we need some conditions on the lattice. One idea to show the uniqueness was shown by Lieb.[48]. Let us define a positive semidefinite matrix $R = P - C$ and show that $R = 0$. Since R can be regarded as a map $R : X^{\downarrow} \to X^{\uparrow}$, $R = 0$

means that $Rv = 0$ for every $v \in X^{\downarrow}$, i.e. $K \equiv \{v \in X^{\downarrow} | Rv = 0\} = X^{\downarrow}$. If all the eigenvalues have the same sign, $C = \pm P$ holds and we have nothing to prove. Thus, we assume that $C \neq -P$. Then R has at least one zero eigenvalue, indicating that there is an eigenvector v such that $Rv = 0$ for some $v \in X^{\downarrow}$. Because P also satisfies the Schrödinger equation (P is the wave function of the ground state), we obtain for R,

$$K^{\uparrow} R + R K^{\downarrow\dagger} + g \sum_a V_a^{\uparrow} R V_a^{\downarrow\dagger} = ER. \tag{25}$$

From $Rv = 0$, it follows that

$$\sum_a \langle v | V_a^{\uparrow} R V_a^{\downarrow\dagger} | v \rangle = 0. \tag{26}$$

Because of the up-down symmetry, we have

$$\langle v | V_a^{\uparrow} R V_a^{\downarrow\dagger} | V \rangle = \langle v | V_a^{\downarrow} R V_a^{\downarrow\dagger} | v \rangle = \sum_{\alpha} r_{\alpha} |\langle v | V_a^{\downarrow} | \alpha \rangle|^2 \geq 0, \tag{27}$$

where $r_{\alpha} = |\epsilon_{\alpha}| - \epsilon_{\alpha} geq 0$. Therefore $\langle v | V_a^{\downarrow} R V_a^{\downarrow\dagger} | v \rangle = 0$ for any a. Since R is positive semidefinite, one can write $\langle v_a | v_a \rangle = 0$ for $v_a = R^{1/2} V_a^{\downarrow\dagger} | v \rangle$ where $R^{1/2}$ is uniquely determined. Then we obtain $v_a = 0$ which implies

$$R V_a^{\downarrow\dagger} | v \rangle = \langle v | V_a^{\uparrow} R = 0. \tag{28}$$

Now

$$R K^{\downarrow\dagger} | v \rangle = 0 \tag{29}$$

is also followed. For the Hubbard model, $K^{\downarrow}$ is the kinetic energy term and $V_a^{\downarrow}$ are given by a matrix of number operators $n_{i\downarrow}$. In this case, if we assume the connectivity of the lattice, we can create every vector in $X^{\downarrow}$ by succesive application of $K^{\downarrow\dagger}$ and $V_i^{\downarrow\dagger}$ ($i \in \Lambda$) starting from a any vector $v \in X^{\downarrow}$. Thus we have $K = \{v \in X^{\downarrow} | Rv = 0\} = X^{\downarrow}$ and then $R = 0$, i.e. $P = C$. This will prove the uniqueness for the following reason. If there are two normalized ground state C_1 and C_2 with $C_1 \neq C_2$, then for every real constatnt α, the hermitian matrix $C_1 + \alpha C_2$ ($\neq 0$) represents a ground state. We can choose α so that $C_1 + \alpha C_2$ is never positive (or negative) semidefinite. This contradicts the property that the ground state $C_1 + \alpha C_2$ should be positive semidefinite.

We have shown the outline of a proof to show the uniqueness of the ground state. We have two steps; first we show an equality (1) $E(C) = E(P)$ and second, one has to show (2) $C = P$ (or $C = -P$). The negative $g < 0$ means an attractive interaction for the Hubbard model. Therefore, the method is strictly restricted to models where the interaction is attractive or can be transformed into attractive one by some transformations which preserve the up-down symmetry.

Let us mention that we cannot predict the total spin of the ground state within the theory of positive semidefinite matrix without exceptional cases. In many cases we can only show that the ground state is unique and we should refer to other methods, for example, the Perron-Frobenius theorem, to obtain the total spin S.

2.2. *The negative-U Hubbard model*

As a first example, let us consider the Hubbard model with the negative Coulomb interactions, which is given as

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{30}$$

where $c_{i\sigma}(c^{\dagger}_{i\sigma})$ denote annihilation (creation) operators of the conduction electrons. The Coulomb interaction parameter U is assumed to be negative ($U < 0$). We also assume that the number of electrons is even. Let us denote the lattice on which the Hamiltonian is defined as Λ.

Definition A lattice Λ is said to be connected with respect to $\{t_{ij}\}$ if there is a connected path of bonds by $\{t_{ij}\}$ between every pair of sites: for any $i, j \in \Lambda$, $t_{ij} \neq 0$ or there is a set of sites $\{i_1, \cdots, i_n\} \subset \Lambda$ such that $t_{ii_1} t_{i_1 i_2} \cdots t_{i_{n-1} i_n} t_{i_n j} \neq 0$.

The theorem obtained by Lieb is written as:

Theorem 2.1 We assume that Λ is connected and we have an even number of electrons. Then the ground state of the Hubbard model is unique for any negative $U < 0$ and has $S = 0$.

Remarks No other conditions on t_{ij} are needed. Since the Hamiltonian is isotropic in the spin space, we can work in the subspace $S^z = 0$. Let $\{\psi_{\alpha\beta} = \psi^{\uparrow}_{\alpha} \otimes \psi^{\downarrow}_{\beta}\}$ be a set of real basis states within the subspace $S^z = 0$. The ground state wave function is written as $\psi = \sum_{\alpha\beta} C_{\alpha\beta} \psi_{\alpha\beta}$ as is shown in the preceeding section.

Proof The expectation value of the Hamiltonian is written as

$$E(C) = Tr(C^{\dagger} K^{\uparrow} C + C K^{\downarrow} C^{\dagger}) + U \sum_{i} Tr C^{\dagger} N^{\uparrow}_{i} C N^{\downarrow}_{i}, \tag{31}$$

where matrices are defined as

$$(K^{\sigma})_{\alpha\beta} = \langle \psi^{\sigma}_{\alpha} | - \sum_{ij} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} | \psi^{\sigma}_{\beta} \rangle, \tag{32}$$

$$(N^{\sigma}_{i})_{\alpha\beta} = \langle \psi^{\sigma}_{\alpha} | n_{i\sigma} | \psi^{\sigma}_{\beta} \rangle. \tag{33}$$

K^{σ} and N^{σ}_{i} are real symmetric matrices. According to the up-down symmetry, we have $K^{\uparrow} = K^{\downarrow}$ and $N^{\uparrow}_{i} = N^{\downarrow}_{i}$. Hence C can be assumed to be hermitian from eqs.(16) and (17). Now we can apply the Schwarz inequality

$$Tr C^{\dagger} N^{\uparrow}_{i} C N^{\downarrow}_{i} \leq Tr P N^{\uparrow}_{i} P N^{\downarrow}_{i}, \tag{34}$$

to $E(C)$ and obtain

$$E(C) \geq E(P), \tag{35}$$

for $U < 0$ where P is the positive semidefinite matrix defined by eq.(22): $P = (C^\dagger C)^{1/2}$. If we assume that ψ is the ground state, we have $E(C) = E(P)$. Then $C = P$ (or $C = -P$) is a solution of this equation. In order to show a uniqueness of the ground state, we define $R = P - C$ following the outline in **2.1** and show that $\mathrm{Ker}R \equiv \{v \in X^\downarrow | Rv = 0\} = X^\downarrow$. First, note that R satisfies

$$K^\uparrow R + RK^\downarrow + U\sum_i N_i^\uparrow R N_i^\downarrow = ER. \tag{36}$$

R has at least one eigenvector which belongs to zero eigenvalue: $Rv = 0$ (otherwise we have $P = -C$.) From eq.(36), we obtain

$$\langle v| \sum_i N_i R N_i |v\rangle = 0, \tag{37}$$

where $N_i \equiv N_i^\downarrow = N_i^\uparrow$. Since R is positive semidefinite, $RN_i^\downarrow v = 0 (\forall i)$ are followed. This implies $RK^\downarrow v = 0$. Then we can show that by successive application of $N_i^\downarrow$ and $K^\downarrow$, one can construct every vector starting from v in the space $X^\downarrow$. In order to see this, let us write an initial vector in the form,

$$v = c^\dagger_{i_1\downarrow} c^\dagger_{i_2\downarrow} \cdots c^\dagger_{i_{N_e/2}\downarrow} |0\rangle. \tag{38}$$

If we want to move an electron on the site i_1, we apply operators $N_{i_2}^\downarrow \cdots N_{i_{N_e/2}}^\downarrow K^\downarrow$ to v. In order to fix a direction of transfer, we further apply $N_j^\downarrow$ where j is a site connected to i_1 by the kinetic term. Repeating this procedure, we can construct all the vectors in $X^\downarrow$, which is guaranteed by the connectivity of t_{ij} on the lattice. Then we can show that $C = P$ is a unique solution of $E(C) = E(P)$, which concludes the uniqueness of the ground state. Therefore the ground state is connected for all $U < 0$ and unique without level crossings with respect to $U(< 0)$. In the limit $-U \to \infty$, the ground state has clearly $S = 0$. Or we can make the following discussion. Since C is positive semidefinite now, $TrC = \sum_\alpha \epsilon_\alpha > 0$ (if $TrC = 0$, then $C = 0$). Thus we have $C_{\alpha\alpha} \neq 0$ for some α. $\psi_{\alpha\alpha}$ is the basis state which has only the double occupied sites and obviously has $S = 0$. □

The proof of *Theorem 2.1* leads to a stronger statement.

Corollary Under the assumptions of the *Theorem 2.1*, the coefficient matrix C of the ground state is strictly positive definite.

Proof We have shown that C is positive semidefinite. Let us assume that C has a vanishing eigenvalue ϵ_1. Then $v = U^\dagger(1, 0, \cdots, 0)^t$ (where U is a unitary matrix in eq.(20)) satisfies $Rv = 0$ for $R = P - C$. This means that $\mathrm{Ker}R = X^\downarrow$ and $P = C$. Similarly, we obtain $Sv = 0$ for $S = P + C$ and then $P = -C$ is followed. Thus we have $C = -C$; i.e. $C = 0$. This is a contradiction. (The ground state should be non-trivial $C \neq 0$.) Hence C has no zero eigenvalues and then is positive definite. □

It is obvious that we can generalize the Hamiltonian where the strength of attractive force is site dependent $U_i < 0$.

2.3. *The Hubbard model at half filling*

An attractive interaction is essential to apply the Schwarz inequality to the energy expectation value. If we remember that the repulsive Hubbard model

$$H = -\sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{39}$$

can be transformed to an attractive one by the electron-hole transformation for the half-filled case,[55,56] the positive semidefinite matrix method is also applicable to the repulsive model.

Definition A lattice Λ is said to be bipartite with respect to $\{t_{ij}\}$ if Λ is divided into two disjoint sublattices A and B such that $t_{ij} = 0$ for $i \in A$ and $j \in A$ or $i \in B$ and $j \in B$. Conventionally, we say that a lattice is bipartite if this condition holds.

We should assume that the lattice Λ is bipartite. The following statement is important.[48]

Theorem 2.2 Let us assume that Λ is bipartite and connected with respect to $\{t_{ij}\}$. The number of electrons N_e is equal to the number of the lattice $|\Lambda|$. We further assume that N_e is even. Then the ground state of the Hubbard model for $U > 0$ is unique apart from a trivial degeneracy due to S^z.

Proof We have included the chemical potential $\mu = U/2$ so as to consider the half-filled case. We work in the space $S^z = 0$. First we make the partial elecron-hole transformation for the down spin: $c_{i\downarrow} \to c_{i\downarrow}^{\dagger}, c_{i\downarrow}^{\dagger} \to c_{i\downarrow}$ for $i \in A$ and $c_{i\downarrow} \to -c_{i\downarrow}^{\dagger}, c_{i\downarrow}^{\dagger} \to -c_{i\downarrow}$ for $i \in B$. The up spins are unaltered. Then the Hamiltonian is transformed to

$$\tilde{H} = -\sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \mu \sum_{i\sigma} n_{i\sigma} - U \sum_{i} n_{i\uparrow} n_{i\downarrow}. \tag{40}$$

We denote the number operators as $N_\sigma = \sum_i n_{i\sigma}$. They transform as $N_\uparrow \to N_\uparrow$ and $N_\downarrow \to |\Lambda| - N_\downarrow$. The condition $N_\uparrow + N_\downarrow = |\Lambda|$ becomes $N_\uparrow = N_\downarrow$ in the new system. The spin operators transform as

$$S^z = \frac{1}{2}(N_\uparrow - N_\downarrow) \to J^z \equiv \frac{1}{2}(N^\uparrow + N^\downarrow - |\Lambda|), \tag{41}$$

$$S^+ = \sum_i c_{i\uparrow}^{\dagger} c_{i\downarrow} \to \eta^{\dagger} \equiv \sum_i \epsilon_i c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger}, \tag{42}$$

$$S^- = \sum_i c_{i\downarrow}^{\dagger} c_{i\uparrow} \to \eta = \sum_i \epsilon_i c_{i\downarrow} c_{i\uparrow}, \tag{43}$$

$$\mathbf{S}^2 \to \mathbf{J}^2 \equiv \frac{1}{2}(\eta^\dagger\eta + \eta\eta^\dagger) + (J^z)^2, \tag{44}$$

where $\epsilon_i = 1$ for $i \in A$ and $\epsilon_i = -1$ for $i \in B$. η operators commute with $\tilde{H}$, and the z-component of the total spin is transformed to $J^z = 0$. The ground-state wave function is written as $\psi = \sum_{\alpha\beta} C_{\alpha\beta}\psi_{\alpha\beta}$ and the expectation value of $\tilde{H}$ is given by

$$\begin{aligned} E(C) &= Tr(C^\dagger K^\uparrow C + CK^\downarrow C^\dagger) + \mu \sum_i Tr(C^\dagger N_i^\uparrow C + CN_i^\downarrow C^\dagger) \\ &- U \sum_i Tr C^\dagger N_i^\uparrow C N_i^\downarrow. \end{aligned} \tag{45}$$

We can assume the up-down symmetry $K^\uparrow = K^\downarrow$ and $N_i^\uparrow = N_i^\downarrow$, and then C is assumed to be hermitian. Therefore the energy inquality holds: $E(C) \geq E(P)$. Now the same method as in *Theorem 2.1* proves *Theorem 2.2*.□

Clearly we can repeat the same arguments in the subspace $S^z = 0, 1, \cdots, |\Lambda|/2$ (when $|\Lambda|$ is assumed to be even). Hence in each subspace with definite values of S^z, we can proove the uniqueness of lowest energy state. It should be noted that C is shown to be strictly positive definite as is in *Corollary* of *Theorem 2.1*.

In *Theorem 2.2* we have assumed that $|\Lambda| = N_e$ is even.[48] This condition can be relaxed since the proof is also relevant when $|\Lambda|$ is odd. We work in the subspace $S^z = 1/2$ for odd $|\Lambda|$. After the electron-hole transformation for the up-spin electrons, our model is transformed to the negative-U Hubbard model with an even number of electrons. Hence we can say in the following way.

Theorem 2.2' Let us assume that Λ is bipartite and connected with respect to $\{t_{ij}\}$. The number of electrons N_e is equal to the number of the lattice $|\Lambda|$. Then the ground state of the Hubbard model for $U > 0$ is unique apart from a trivial degeneracy due to S^z.

In order to determine the total spin of the ground state, we take the limit $U \to \infty$. In the large-U case, the original Hamiltonian is transformed onto the Heisenberg model. For the spin-1/2 Heisenberg on a bipartite lattice, the signs of coefficients $C_{\alpha\beta}$ in the ground state are uniquely determined. Mathematically, this is proved by the Perron-Frobenius theorem in matrix theory. This fact will lead us to determine the total spin of the ground state, which is a theorem given by Lieb and Mattis:[57]

Lemma 2.3 Let us consider the spin-1/2 antiferromagnetic Heisenberg model on a connected and bipartite lattice,

$$H_A = \sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{46}$$

where J_{ij} are non-zero for $i \in A$ and $j \in B$ or $i \in B$ and $j \in A$. Let us denote the number of sites in A and B sublattices as $|A|$ and $|B|$, respectively, and assume

that $|A| \geq |B|$. Then the ground state of H_A has $S = (|A| - |B|)/2$.

According to this Lemma, we can say that

Corollary We assume that the same conditions for the Hubbard model with $U > 0$ at half filling. Then the ground state has $S = (|A| - |B|)/2$.

Therefore we have a ferromagnetic state for $|A| > |B|$. This ferromagnetism (more correctly, ferrimagnetism) should be understood in the sense that the total spin is proportional to the number of electrons. A two-dimensional model in high-T_c oxide superconductors provide us an example of a model of ferromagnetism. The non-interacting case has three bands which are bonding, non-bonding, and anti-bonding bands. The half-filled case has electrons in the non-bonding dispersionless band, which supports the ferromagnetism. It is quite likely that this model describes an insulator.

Since the lowest energy state is unique in each subspace with definite value of S^z, inequalities $E_g(S) < E_g(S+1)$ holds for $S \geq (|A| - |B|)/2$ where $E_g(S)$ is the lowest energy with the total spin S.[57]

It is easy to see that we can replace the Coulomb interactions by the site-dependent ones $\sum_i U_i n_{i\uparrow} n_{i\downarrow}$ as fas as $U_i > 0$ $(\forall i)$. One can also include the site-dependent one-body term such as $\sum_i \epsilon_i n_{i\sigma}$ as far as $\epsilon_i = -U_i/2$. This observation leads us to investigate the (periodic) Anderson model. Let us consider the periodic Anderson model given as

$$\begin{aligned} H &= -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} n_{ci\sigma} + U \sum_i n_{ci\uparrow} n_{ci\downarrow} \\ &+ V \sum_{i\sigma} (c^\dagger_{i\sigma} f_{i\sigma} + h.c.) + \epsilon_f \sum_{i\sigma} n_{fi\sigma} + U_f \sum_i n_{fi\uparrow} n_{fi\downarrow}, \end{aligned} \tag{47}$$

where $f_{i\sigma}(f^\dagger_{i\sigma})$ denote operators of the localized electrons and we write $n_{fi\sigma} = f^\dagger_{i\sigma} f_{i\sigma}$ and $n_{ci\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. We set $\epsilon_f = -U_f/2$ (symmetric case). $\langle ij \rangle$ indicates a nearest-neighbor pair of sites. The last term indicates the Coulomb interaction between the f electrons, and the fourth term drives hybridization processes between the conduction electrons and localized electrons. This model has been investigated by many methods such as numerical calculations[59,60,61,62], variational theory,[63,64,65,66,67,68,69,70,71,72] and renormalized band theory.[73] A slight extension of *Theorem 2.2* proves the following theorem.[58]

Theorem 2.4 Let us consider the symmetric Anderson model on a bipartite and connected lattice where the total lattice including both the conduction and f electrons is bipartite. The lattice of the conduction electrons is also bipartite itself where t_{ij} are assumed to be zero for $i, j \in A$ or $i, j \in B$. We examine the half-filled case in which we set $\mu = U/2$ and $\epsilon_f = -U_f/2$. Then the ground state of the symmetric periodic Anderson model is unique for $U > 0$ and $U_f > 0$, and has

$S = 0$.

Proof We again make the electron-hole transformation for the down spin: $c_{i\downarrow} \to c^\dagger_{i\downarrow}$ and $c^\dagger_{i\downarrow} \to c_{i\downarrow}$ for $i \in A$, $c_{j\downarrow} \to -c^\dagger_{j\downarrow}$ and $c^\dagger_{j\downarrow} \to -c_{j\downarrow}$ for $j \in B$, $f_{i\downarrow} \to -f^\dagger_{i\downarrow}$ and $f^\dagger_{i\downarrow} \to -f_{i\downarrow}$ for $i \in A$, and $f_{j\downarrow} \to f^\dagger_{j\downarrow}$ and $f^\dagger_{j\downarrow} \to f_{j\downarrow}$ for $j \in B$. The up electrons are unaltered. Then the Hamiltonian is transformed into

$$\begin{aligned} \tilde{H} &= -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mu \sum_{i\sigma} n_{i\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow} \\ &+ V \sum_{i\sigma} (c^\dagger_{i\sigma} f_{i\sigma} + h.c.) - \epsilon_f \sum_{i\sigma} n_{fi\sigma} - U_f \sum_i n_{fi\uparrow} n_{fi\downarrow}. \end{aligned} \tag{48}$$

We can apply a same argument to show a uniqueness of the ground state for $U > 0$ and $U_f > 0$. In order to predict the value of total spin, let us consider the strong-U and -U_f limit where the system is represented by an antiferromagnetic Heisenberg model. Since we have the same number of sites in A and B sublattices, the ground state should have $S = 0$. □

Because we have a finite energy gap for the non-interacting case, we can expect a finite gap for $U_f > 0$. However, there is no proof for this expectation.

It is also straightforward to investigate single-impurity Anderson model, two-impurity model, or other variants of the Anderson model as a slight modification of *Theorem 2.4*. The two-impurity Anderson model is a simplest non-trivial extension of the single-impurity Anderson model.[74,75,76,77,78,79,80,81,82] It is quite likely that this model contains competition effects between the local Kondo effect and the intersite (RKKY) interaction. According to the *Theorem 2.2* and the *Corollary*, the interspin interaction is an oscillating function of the distance d between two localized spins since the ground state has $S = 0$ for even d and $S = 1$ for odd d (in units of the lattice constant) at half filling (where we assume that the lattice for the conduction electrons have the same number of sites in A and B sublattices).

2.4. *Heisenberg model*

Since the antiferromagnetic Heisenberg model is obtained as the large-U limit in the Hubbard model, it may be clear that the Heisenberg model has a positive semidefinite matrix for the ground state. Although the uniqueness of the ground state for the Heisenberg model is established,[57] we discuss the positivity of the coefficient matrix here since we can apply our technique to the Kondo lattice which will be discussed in the next section. Let us consider the following proposition:[83]

Theorem 2.5 Let us consider the antiferromagnetic Heisenberg model given as

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{49}$$

on a bipartite lattice $|\Lambda|$ with respect to $\{J_{ij} \geq 0\}$. We assume that $|\Lambda|$ is connected with respect to $\{J_{ij}\}$. Then, the ground state has a positive semidefinite coefficient

matrix (after a electron-hole transformation) and is unique.

Proof We write the Hamiltonian by fermions as follows.

$$\begin{aligned} H &= \sum_{ij} J_{ij}[\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z] \\ &= \sum_{ij} J_{ij}[\frac{1}{2}(c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{i\uparrow} c_{j\uparrow}^\dagger c_{j\downarrow}) + \frac{1}{4}(n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow})], \quad (50) \end{aligned}$$

where $c_{i\sigma}$ ($c_{i\sigma}^\dagger$) denote fermion operators of localized electrons and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. Since we have always one spin at each site, we impose the constraint $n_{i\uparrow} + n_{i\downarrow} = 1$. Now we make the electron-hole transformation for down spins: $c_{i\downarrow} \to c_{i\downarrow}^\dagger$ and $c_{i\downarrow}^\dagger \to c_{i\downarrow}$ for $i \in A$, and $c_{j\downarrow} \to -c_{j\downarrow}^\dagger$ and $c_{j\downarrow}^\dagger \to -c_{j\downarrow}$ for $j \in B$. Then the transformed Hamiltonian is written as

$$\tilde{H} = \sum_{ij} J_{ij}[-\frac{1}{2}(c_{i\uparrow}^\dagger c_{j\uparrow} c_{i\downarrow}^\dagger c_{j\downarrow} + c_{j\uparrow}^\dagger c_{i\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow}) + \frac{1}{4}(n_{i\uparrow} + n_{i\downarrow} - 1)(n_{j\uparrow} + n_{j\downarrow} - 1)], \quad (51)$$

where the constraint is given as $n_{i\uparrow} = n_{i\downarrow}$. We set $Q_i = n_{i\uparrow} - n_{i\downarrow}$. It is easy to see that Q_i commutes with $\tilde{H}$ and Q_j each other:

$$[Q_i, \tilde{H}] = 0, [Q_i, Q_j] = 0 (\forall i, j \in \Lambda). \quad (52)$$

Then the total space of configurations is divided into subspaces which are specified by eigenvalues of Q_i. Obviously the subspace given by

$$S_0 \equiv \{\psi (\neq 0) | Q_i \psi = 0 (\forall i)\} \quad (53)$$

is the physical subspace. In this subspace, eigenfunctions satisfy

$$\tilde{H}\psi = E\psi, \quad (54)$$

$$Q_i \psi = 0. \quad (55)$$

Let us again express the ground-state wave function in a form $\psi = \sum_{\alpha\beta} C_{\alpha\beta} \psi_{\alpha\beta}$ with real basis states $\{\psi_{\alpha\beta}\}$. According to eqs.(12), (13), and (14), the Schrödinger equation (54) reads

$$\begin{aligned} EC &= \sum_{ij} J_{ij}[-\frac{1}{2}(T_{ij}^\uparrow C T_{ij}^{\downarrow\dagger} + T_{ji}^\uparrow C T_{ji}^{\downarrow\dagger}) + \frac{1}{4}(N_{ij}^\uparrow C + C N_{ij}^{\downarrow\dagger}) \\ &+ \frac{1}{4}(N_i^\uparrow C N_j^{\downarrow\dagger} + N_j^\uparrow C N_i^{\downarrow\dagger}) - \frac{1}{4}(N_i^\uparrow C + N_j^\uparrow C + C N_i^{\downarrow\dagger} + C N_j^{\downarrow\dagger})], \quad (56) \end{aligned}$$

and the constraint equations are written as

$$N_i^\uparrow C = C N_i^\downarrow, \quad (57)$$

where matrices are defined by the following:

$$(T_{ij}^{\sigma})_{\alpha\alpha'} = \langle\psi_{\alpha}^{\sigma}|c_{i\sigma}^{\dagger}c_{j\sigma}|\psi_{\alpha'}^{\sigma}\rangle, \tag{58}$$

$$(N_{ij}^{\sigma})_{\alpha\alpha'} = \langle\psi_{\alpha}^{\sigma}|n_{i\sigma}n_{j\sigma}|\psi_{\alpha'}^{\sigma}\rangle, \tag{59}$$

$$(N_{i}^{\sigma})_{\alpha\alpha'} = \langle\psi_{\alpha}^{\sigma}|n_{i\sigma}|\psi_{\alpha'}^{\sigma}\rangle. \tag{60}$$

The up-down symmetry implies $T_{ij}^{\uparrow} = T_{ij}^{\downarrow}$, $N_{ij}^{\uparrow} = N_{ij}^{\downarrow}$ and $N_{i}^{\uparrow} = N_{i}^{\downarrow}$. $(N_{ij}^{\sigma})^{\dagger} = N_{ij}^{\sigma}$ and $(N_{i}^{\sigma})^{\dagger} = N_{i}^{\sigma}$ are obvious. Then we can assume that C is hermitian. From eq.(56), the energy-expectation value is easily calculated as

$$\begin{aligned} E(C) &= \sum_{ij} J_{ij}[-\frac{1}{2}Tr(C^{\dagger}T_{ij}^{\uparrow}CT_{ij}^{\downarrow\dagger} + C^{\dagger}T_{ji}^{\uparrow}CT_{ji}^{\downarrow\dagger}) + \frac{1}{4}Tr(C^{\dagger}N_{ij}^{\uparrow}C + CN_{ij}^{\downarrow}C^{\dagger}) \\ &+ \frac{1}{4}Tr(C^{\dagger}N_{i}^{\uparrow}CN_{j}^{\downarrow} + C^{\dagger}N_{j}^{\uparrow}CN_{i}^{\downarrow}) - \frac{1}{4}Tr(C^{\dagger}N_{i}^{\uparrow}C + C^{\dagger}N_{j}^{\uparrow}C \\ &+ CN_{i}^{\downarrow}C^{\dagger} + CN_{j}^{\downarrow}C^{\dagger})]. \end{aligned} \tag{61}$$

Here we use the constraint equations $N_{i}^{\uparrow}C = CN_{i}^{\downarrow}$ to get

$$TrC^{\dagger}N_{i}^{\uparrow}CN_{j}^{\downarrow} = TrC^{\dagger}N_{i}^{\uparrow}N_{j}^{\uparrow}C = TrC^{\dagger}N_{ij}^{\uparrow}C, \tag{62}$$

and we write the energy $E(C)$ as

$$\begin{aligned} E(C) &= \sum_{ij} J_{ij}[-\frac{1}{2}Tr(C^{\dagger}T_{ij}^{\uparrow}CT_{ij}^{\downarrow\dagger} + C^{\dagger}T_{ji}^{\uparrow}CT_{ji}^{\downarrow\dagger}) + \frac{1}{2}Tr(C^{\dagger}N_{ij}^{\uparrow}C + CN_{ij}^{\downarrow}C^{\dagger}) \\ &- \frac{1}{4}Tr(C^{\dagger}N_{i}^{\uparrow}C + C^{\dagger}N_{j}^{\uparrow}C + CN_{i}^{\downarrow}C^{\dagger} + CN_{j}^{\downarrow}C^{\dagger})]. \end{aligned} \tag{63}$$

Therefore one can make use of the Schwarz inequality to obtain

$$E(C) \geq E(P), \tag{64}$$

where P is the positive semidefinite matrix which satisfies $P^2 = C^{\dagger}C = CC^{\dagger}$. Here we must show that the wave function with the coefficient matrix P also belongs to the physical subspace S_0, which means that $PN_{i}^{\downarrow} = N_{i}^{\uparrow}P$ (for all $i \in \Lambda$). This constraint indicates that we have no singly occupied sites in fermion representation which means $\langle n_{i\uparrow}(1-n_{i\downarrow})\rangle_P \equiv \mathrm{Tr}PN_{i\uparrow}P(1-N_{i\downarrow}) = 0$ and $\langle n_{i\downarrow}(1-n_{i\uparrow})\rangle_P \equiv \mathrm{Tr}PN_{i\downarrow}P(1-N_{i\uparrow}) = 0$. According to the Schwarz inequality $TrCN_{i}^{\uparrow}C^{\dagger}N_{i}^{\downarrow} \leq TrPN_{i}^{\uparrow}PN_{i}^{\downarrow}$, we obtain

$$\begin{aligned} 0 &\leq TrPN_{i}^{\uparrow}P(1-N_{i}^{\downarrow}) = TrPN_{i}^{\uparrow}P - TrPN_{i}^{\uparrow}PN_{i}^{\downarrow} \\ &\leq TrCN_{i}^{\uparrow}C - TrCN_{i}^{\uparrow}CN_{i}^{\downarrow} = TrCN_{i}^{\uparrow}C(1-N_{i}^{\downarrow}) = 0, \end{aligned} \tag{65}$$

where we note that $TrCN_{i}^{\uparrow}C(1-N_{i}^{\downarrow}) = TrCN_{i}^{\uparrow}(1-N_{i}^{\uparrow})C = 0$ because of $N_{i}^{\uparrow}C = CN_{i}^{\downarrow}$ and $(N_{i}^{\sigma})^2C = N_{i}^{\sigma}C$ (which follows from $n_{i\sigma}^2\psi = n_{i\sigma}\psi$). Now it is followed that $TrPN_{i}^{\uparrow}P(1-N_{i}^{\downarrow}) = 0$. Since we have also $(N_{i}^{\sigma})^2P = N_{i}^{\sigma}P$, one gets

$$TrPN_{i}^{\uparrow}P(1-N_{i}^{\downarrow}) = Tr(1-N_{i}^{\downarrow})PN_{i}^{\uparrow}N_{i}^{\uparrow}P(1-N_{i}^{\downarrow}) = ||N_{i}^{\uparrow}P(1-N_{i}^{\downarrow})||^2 = 0, \tag{66}$$

where the norm $||\cdot||$ is defined by $||A|| = (TrA^\dagger A)^{1/2}$. This implies $N_i^\uparrow P(1-N_i^\downarrow) = 0$. Similarly we can obtain $(1-N_i^\uparrow)PN_i^\downarrow = 0$. Therefore the constrain equation is followed:

$$N_i^\uparrow P = PN_i^\downarrow. \tag{67}$$

Now the energy equality $E(C) = E(P)$ has its sense. Following the same arguments as before, the uniqueness of the ground state is proved, i.e. $C = P$ (or $C = -P$) is a unique solution for the ground-state wave function. □

Remarks The above proof consists of three steps: (I) To show the inequality $E(C) \geq E(P)$ for $\psi(C) \in S_0$, (II) To show $\psi(P) \in S_0$, and (III) To show that $C = P$ (or $C = -P$) is a unique solution of $E(C) = E(P)$. Here we have used the Schwarz inequality to show the step (II).

Thus the semidefinite positivity of the ground state wave function is rather instinsic for the antiferromagnetic Heisenberg model. We should refer to the other method (for example, the Perron-Frobenius theorem) to predict the total spin of the ground state, which we shall discuss in the next Chapter. However, it is easy to see that the ground state has $S = 0$ if two sublattices A and B have the same number of sites because we clearly have $S = 0$ in the limit of large $J_{ij} > 0$. Next we comment on a similar theorem for the ferromagnetic Heisenberg model, which is rather trivial since we obviously have a unique ferromagnetic ground state.

Theorem 2.6 Let us consider the ferromagnetic Heisenberg model on a connected lattice Λ:

$$H = \sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{68}$$

where non-zero J_{ij} are negative: $J_{ij} < 0$. Then the ground state has a positive semidefinite coefficient matrix and is unique.

Proof Let us make again a partial electron-hole transformation for the down spin in a fermion representation: $c_{i\downarrow} \to c_{i\downarrow}^\dagger$ and $c_{i\downarrow}^\dagger \to c_{i\downarrow}$ for $i \in \Lambda$. The Hamiltonian is transformed into

$$\begin{aligned} \tilde{H} &= \sum_{ij} J_{ij}[\frac{1}{2}(c_{i\uparrow}^\dagger c_{j\uparrow} c_{i\downarrow}^\dagger c_{j\downarrow} + c_{i\uparrow}c_{j\uparrow}^\dagger c_{i\downarrow}c_{j\downarrow}^\dagger) \\ &+ \frac{1}{4}(n_{i\uparrow} + n_{i\downarrow} - 1)(n_{j\uparrow} + n_{j\downarrow} - 1)], \end{aligned} \tag{69}$$

where we must impose $n_{i\uparrow} = n_{i\downarrow}$ for wave functions. Now it is obvious that the same argument will conclude the proof since the energy-expectation value is written as

$$\begin{aligned} E(C) &= \sum_{ij} J_{ij}[\frac{1}{2}Tr(C^\dagger T_{ij}^\uparrow C T_{ij}^{\downarrow\dagger} + C^\dagger T_{ji}^\uparrow C T_{ji}^{\downarrow\dagger}) + \frac{1}{2}Tr(C^\dagger N_{ij}^\uparrow C + C N_{ij}^\downarrow C^\dagger) \\ &- \frac{1}{4}Tr(C^\dagger N_i^\uparrow C + C^\dagger N_j^\uparrow C + C N_i^\downarrow C^\dagger + C N_j^\downarrow C^\dagger)], \end{aligned} \tag{70}$$

and we can derive $E(C) \geq E(P)$. The constraint equations are proved for P in the same way as in *Theorem 2.5.* □

These theorems for the Heisenberg model may be proved by other method in a more elegant way. Our proof will give a way to consider more complicated models such as the Kondo lattice or the Kondo-Hubbard Hamiltonians, which are going to be discussed in the next sections.

2.5. *Kondo lattice Hamiltoninan*

Let us turn to the Kondo lattice Hamiltonian which represents interactions between the localized spins and the conduction electrons. The model is written as

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} - \mu \sum_{i} n_{ci\sigma} + U \sum_{i} n_{ci\uparrow} n_{ci\downarrow} + J \sum_{i} \mathbf{S}_i \cdot \sigma_i, \tag{71}$$

where $c_{i\sigma}$ ($c^{\dagger}_{i\sigma}$) denote annihilation (creation) operators of the conduction electrons and we write $n_{ci\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. The third term shows the Coulomb interactions between the conduction electrons and the last term represents the exchange interactions where $\mathbf{S}_i$ and σ_i denote spin operators of the localized spins and the conduction electrons, respectively. We have localized spins on each site in the Kondo lattice Hamiltonian. We assume repulsive Coulomb interactions $U > 0$. Note that the Kondo lattice model is usually defined without Coulomb interaction U. Here we include the Coulomb terms in order to show a uniqueness of the ground state. Let us consider a bipartite lattice Λ with respect to $\{t_{ij}\}$ and fix the number of electrons to be $|\Lambda|$ (half-filled case), i.e. $\mu = U/2$. We first investigate the antiferromagnetic exchange interaction $J > 0$.[83]

Theorem 2.7 Let us consider the Kondo lattice Hamiltonian in eq.(71) for $U > 0$ and $J > 0$ at half filling. We assume that the lattice is bipartite where hopping parameters t_{ij} are nonzero for $i \in A$ and $j \in B$ or $i \in B$ and $j \in A$. The connectivity of the lattice due to t_{ij} is also assumed. Then the ground state is unique and has $S = 0$.

Proof Following the proof for the Heisenberg model, we use fermions to express the localized spins and write the Hamiltonian in the form,

$$\begin{aligned} H &= -\sum_{\langle ij\rangle\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i} [\frac{1}{2} J_{\perp} (c^{\dagger}_{i\uparrow} c_{i\downarrow} f^{\dagger}_{i\downarrow} f_{i\uparrow} \\ &+ c^{\dagger}_{i\downarrow} c_{i\uparrow} f^{\dagger}_{i\uparrow} f_{i\downarrow}) + \frac{1}{4} J_z (n_{ci\uparrow} - n_{ci\downarrow})(n_{fi\uparrow} - n_{fi\downarrow})] \\ &+ U \sum_{i} n_{ci\uparrow} n_{ci\downarrow} - \frac{U}{2} \sum_{i\sigma} n_{ci\sigma}, \end{aligned} \tag{72}$$

where $f_{i\sigma}$ ($f^{\dagger}_{i\sigma}$) denote annihilation (creation) operators of localized spins. $n_{fi\sigma}$ indicate the number operator of localized fermions. We have written the perpendicular-

and z-component of exchange interaction as $J_\perp$ and J_z, respectively. Let us assume that $J = J_\perp = J_z$. We make the electron-hole transformation for the up spins: $c_{i\uparrow} \to c^\dagger_{i\uparrow}$, $c^\dagger_{i\uparrow} \to c_{i\uparrow}$ for $i \in A$, $f_{i\uparrow} \to -f^\dagger_{i\uparrow}$, $f^\dagger_{i\uparrow} \to -f_{i\uparrow}$ for $i \in A$ and $c_{i\uparrow} \to -c^\dagger_{i\uparrow}$, $c^\dagger_{i\uparrow} \to -c_{i\uparrow}$ for $i \in B$, $f_{i\uparrow} \to f^\dagger_{i\uparrow}$,$f^\dagger_{i\uparrow} \to f_{i\uparrow}$ for $i \in B$ where we have assumed that the lattice is bipartite-divided into two disjoint sets A and B. The spin-down electrons are unaltered, $c_{i\downarrow} \to c_{i\downarrow}$ and $f_{i\downarrow} \to f_{i\downarrow}$. In this transformation the z-component of the total spin is invariant at half filling: $S^z = 0 \to S^z = 0$. Then H is transformed into

$$\begin{aligned}\tilde{H} &= -\sum_{\langle ij\rangle\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - U\sum_i n_{ci\uparrow} n_{ci\downarrow} + \frac{U}{2}\sum_{i\sigma} n_{ci\sigma} + \sum_i [-\frac{1}{2} J_\perp (c_{i\uparrow} c_{i\downarrow} f^\dagger_{i\downarrow} f^\dagger_{i\uparrow} \\ &+ c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} f_{i\uparrow} f_{i\downarrow}) + \frac{1}{4} J_z (1 - n_{ci\uparrow} - n_{ci\downarrow})(1 - n_{fi\uparrow} - n_{fi\downarrow})]. \end{aligned} \tag{73}$$

We work in the S^z=0 subspace since $\mathbf{S}^2$ and S^z are conserved and every energy eigenvalue has a corresponding eigenfunction in this subspace. For $\tilde{H}$ the constraint should read $n_{fi\uparrow} = n_{fi\downarrow}$. We set $Q_i \equiv n_{fi\uparrow} - n_{fi\downarrow}$. It is easy to see that Q_i commutes with $\tilde{H}$ and Q_j (for any j):

$$[Q_i, \tilde{H}] = 0; [Q_i, Q_j] = 0 (\forall i, j). \tag{74}$$

Therefore the total space is divided into disjoint subspaces which are specified by eigenvalues of Q_i. The physical space is given by $S_0 = \{\psi (\neq 0) | Q_i \psi = 0 (\forall i)\}$.

The Schrödinger equation for C is written in the form,

$$\begin{aligned} EC &= CH^\downarrow_0 + H^\uparrow_0 C - J_\perp \sum_i \frac{1}{2}(M^\uparrow_{fci} C M^\downarrow_{cfi} + M^\uparrow_{cfi} C M^\downarrow_{fci}) \\ &+ J_z \sum_i [\frac{1}{4}(N^\uparrow_{cfi} C + C N^\downarrow_{cfi}) - \frac{1}{4}(C N^\downarrow_{fi} + N^\uparrow_{fi} C) - \frac{1}{4}(C N^\downarrow_{ci} + N^\uparrow_{ci} C) \\ &+ \frac{1}{4}(N^\uparrow_{ci} C N^\downarrow_{fi} + N^\uparrow_{fi} C N^\downarrow_{ci})] - U\sum_i N^\uparrow_{ci} C N^\downarrow_{ci} \\ &+ \frac{U}{2}\sum_i (C N^\downarrow_{ci} + N^\uparrow_{ci} C). \end{aligned} \tag{75}$$

The matrices are defined by the following,

$$(H^\sigma_0)_{\alpha\alpha'} = \langle \psi^\sigma_\alpha | - \sum_{\langle ij\rangle} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} | \psi^\sigma_{\alpha'} \rangle, \tag{76}$$

$$(M^\sigma_{cfi})_{\alpha\alpha'} = \langle \psi^\sigma_\alpha | c^\dagger_{i\sigma} f_{i\sigma} | \psi^\sigma_{\alpha'} \rangle, \tag{77}$$

$$(M^\sigma_{fci})_{\alpha\alpha'} = \langle \psi^\sigma_\alpha | f^\dagger_{i\sigma} c_{i\sigma} | \psi^\sigma_{\alpha'} \rangle, \tag{78}$$

$$(N^\sigma_{cfi})_{\alpha\alpha'} = \langle \psi^\sigma_\alpha | n_{ci\sigma} n_{fi\sigma} | \psi^\sigma_{\alpha'} \rangle, \tag{79}$$

$$(N^\sigma_{ci})_{\alpha\alpha'} = \langle \psi^\sigma_\alpha | n_{ci\sigma} | \psi^\sigma_{\alpha'} \rangle, \tag{80}$$

$$(N^{\sigma}_{fi})_{\alpha\alpha'} = \langle\psi^{\sigma}_{\alpha}|n_{fi\sigma}|\psi^{\sigma}_{\alpha'}\rangle. \tag{81}$$

Please note that these matrices are real ones. From the definition, we have

$$(N^{\sigma}_{cfi})_{\alpha\alpha'} = \sum_{\beta}\langle\psi^{\sigma}_{\alpha}|n_{ci\sigma}|\psi^{\sigma}_{\beta}\rangle\langle\psi^{\sigma}_{\beta}|n_{fi\sigma}|\psi^{\sigma}_{\alpha}\rangle = (N^{\sigma}_{ci}N^{\sigma}_{fi})_{\alpha\alpha'}. \tag{82}$$

We have the up-down symmetry:

$$N^{\sigma}_{ci} = N^{-\sigma}_{ci},\ N^{\sigma}_{fi} = N^{-\sigma}_{fi},\ H^{\sigma}_{0} = H^{-\sigma}_{0}\ and\ M^{\sigma}_{fci} = M^{-\sigma}_{fci}. \tag{83}$$

It is easily followed from eqs(3), (4), and (5) that the constraint equations $Q_i\psi = 0$ is written as

$$N^{\uparrow}_{fi}C = CN^{\downarrow}_{fi}. \tag{84}$$

The energy $E(C)$ is given by

$$\begin{aligned}
E(C) &= Tr(C^{\dagger}H^{\uparrow}_{0}C + CH^{\downarrow}_{0}C^{\dagger}) - J_{\perp}\sum_{i}\frac{1}{2}Tr(M^{\uparrow}_{fci}CM^{\downarrow}_{cfi}C^{\dagger} + M^{\uparrow}_{cfi}CM^{\downarrow}_{fci}C^{\dagger}) \\
&+ J_z\sum_{i}[\frac{1}{4}Tr(C^{\dagger}N^{\uparrow}_{cfi}C + CN^{\downarrow}_{cfi}C^{\dagger}) - \frac{1}{4}Tr(CN^{\downarrow}_{fi}C^{\dagger} + C^{\dagger}N^{\uparrow}_{fi}C) \\
&- \frac{1}{4}Tr(CN^{\downarrow}_{ci}C^{\dagger} + C^{\dagger}N^{\uparrow}_{ci}C) + \frac{1}{4}Tr(N^{\uparrow}_{ci}CN^{\downarrow}_{fi}C^{\dagger} + N^{\uparrow}_{fi}CN^{\downarrow}_{ci}C^{\dagger})] \\
&- U\sum_{i}Tr(N^{\uparrow}_{ci}CN^{\downarrow}_{ci}C^{\dagger}) + \frac{U}{2}\sum_{i}Tr(C^{\dagger}N^{\uparrow}_{ci}C + CN^{\downarrow}_{ci}C^{\dagger}).
\end{aligned} \tag{85}$$

The identity below is useful in the following discussion,[86]

$$\begin{aligned}
J_zTr(C^{\dagger}N^{\uparrow}_{ci}CN^{\downarrow}_{fi} &+ C^{\dagger}N^{\uparrow}_{fi}CN^{\downarrow}_{ci}) \\
&= -J_z\frac{1}{z}TrC^{\dagger}(zN^{\uparrow}_{ci} - N^{\uparrow}_{fi})C(zN^{\downarrow}_{ci} - N^{\downarrow}_{fi}) \\
&+ zJ_zTrC^{\dagger}N^{\uparrow}_{ci}CN^{\downarrow}_{ci} + \frac{1}{z}J_zTrC^{\dagger}N^{\uparrow}_{fi}CN^{\downarrow}_{fi} \\
&= -J_z\frac{1}{z}TrC^{\dagger}(zN^{\uparrow}_{ci} - N^{\uparrow}_{fi})C(zN^{\downarrow}_{ci} - N^{\downarrow}_{fi}) \\
&+ zJ_zTrC^{\dagger}N^{\uparrow}_{ci}CN^{\downarrow}_{ci} + \frac{1}{2z}J_zTr(C^{\dagger}N^{\uparrow}_{fi}C + CN^{\downarrow}_{fi}C^{\dagger}),
\end{aligned} \tag{86}$$

where z is a positive real number $z > 0$ and we have used the relation in eq.(84) to derive the second equality. Then the energy E(C) is written as

$$\begin{aligned}
E(C) &= Tr(C^{\dagger}H^{\uparrow}_{0}C + CH^{\downarrow}_{0}C^{\dagger}) - J_{\perp}\sum_{i}\frac{1}{2}Tr(M^{\uparrow}_{fci}CM^{\downarrow}_{cfi}C^{\dagger} + M^{\uparrow}_{cfi}CM^{\downarrow}_{fci}C^{\dagger}) \\
&+ J_z\sum_{i}[\frac{1}{4}Tr(C^{\dagger}N^{\uparrow}_{cfi}C + CN^{\downarrow}_{cfi}C^{\dagger}) - \frac{1}{4}Tr(CN^{\downarrow}_{fi}C^{\dagger} + C^{\dagger}N^{\uparrow}_{fi}C) \\
&- \frac{1}{4}Tr(CN^{\downarrow}_{ci}C^{\dagger} + C^{\dagger}N^{\uparrow}_{ci}C)]
\end{aligned}$$

$$
\begin{aligned}
&+ \quad \sum_i [-\frac{1}{4z} J_z Tr C^\dagger (z N_{ci}^\uparrow - N_{fi}^\uparrow) C (z N_{ci}^\downarrow - N_{fi}^\downarrow) \\
&+ \quad \frac{1}{4} z J_z Tr C^\dagger N_{ci}^\uparrow C N_{ci}^\downarrow + \frac{1}{8z} J_z Tr (C^\dagger N_{fi}^\uparrow C + C N_{fi}^\downarrow C^\dagger)], \\
&- \quad U \sum_i Tr C^\dagger N_{ci}^\uparrow C N_{ci}^\downarrow + \frac{U}{2} \sum_i Tr (C^\dagger N_{ci}^\uparrow C + C N_{ci}^\downarrow C^\dagger). \qquad (87)
\end{aligned}
$$

Here we can again set that C is hermitian: $C = C^\dagger$ due to the discussion in **2.1**. Then we obtain the inequality $E(C) \geq E(P)$ for $J > 0$ and $U > zJ/4$. Since z is an arbitrary positive real number, we can choose z so that $U > zJ/4$ holds for any positive U. Therefore the inequality $E(C) \geq E(P)$ is followed for every $U > 0$. Since we have assumed that C is the coefficient matrix of the ground state, i.e. $\psi(C)$ is the ground state, we obtain $E(C) = E(P)$. This indicates that there is a state with $C = P$ (or $C = -P$) among the ground states.

Here we should show that $\psi(P)$ belongs to the space S_0: $\psi(P) \in S_0$. In order to show this, we shall prove

$$
N_{fi}^\uparrow P = P N_{fi}^\downarrow, \qquad (88)
$$

which is easily shown by the method in the proceeding section for the Heisenberg model. Thus the equality $E(C) = E(P)$ has its sense.

The uniqueness of the ground state is followed similarly, which means that one can show $\mathrm{Ker}(P - C) = \{v(\neq 0) \in X^\downarrow | (P - C)v = 0\} = X^\downarrow$. Because the energy is continuous with respect to parameters involved in the Hamiltonian, there is no level crossing with respect to $J > 0$. In the large-U limit, H is mapped to a spin-1/2 antiferromagnetic Heisenberg model where we have the same number of sites in two sublattices. Hence the ground state has $S = 0$. □

The method above is also relevant for the Kondo lattice with the ferromagnetic exchange coupling, which is shown as a separate statement.

Theorem 2.8 We consider the Kondo lattice Hamiltonian for $U > 0$ and $J < 0$ at half filling with the same assumptions in *Theorem 2.7*. Then the ground state is unique and has $S = ||A| - |B||$ (where $|A|$ and $|B|$ denote the number of sites in A and B sublattices, respectively).

Proof For $J < 0$, the electron-hole transformation for the down spins are done in the following way: $c_{i\downarrow} \to c_{i\downarrow}^\dagger$, $c_{i\downarrow}^\dagger \to c_{i\downarrow}$ for $i \in A$, $f_{i\downarrow} \to f_{i\downarrow}^\dagger$, $f_{i\downarrow}^\dagger \to f_{i\downarrow}$ for $i \in A$, and $c_{i\downarrow} \to -c_{i\downarrow}^\dagger$, $c_{i\downarrow}^\dagger \to -c_{i\downarrow}$ for $i \in B$, $f_{i\downarrow} \to -f_{i\downarrow}^\dagger$, $f_{i\downarrow}^\dagger \to -f_{i\downarrow}$ for $i \in B$. In order to derive the inequaliy $E(C) \geq E(P)$, we use the identity in eq.(86) with replacing z by $-z$. The total spin of the ground state is easily followed from the formula given by Lieb and Mattis[57] since the Hamiltonian is mapped onto a spin-1 antiferromagnetic Heisenberg model in the limit of large $|J|$. □

Remarks Let us comment on the limit of large $|J|$ ($J < 0$) for the Kondo lattice. Obviously we have local triplets at every site in the limit $|J| = \infty$. Through the virtual states with doubly occupied sites which have higher energies of the order of

$|J|$, the localized spins are exchanged and the degeneracy is lifted. Let us consider the following process

$$\left(\begin{array}{cc} \uparrow & \downarrow \\ \uparrow & \downarrow \end{array} \right) \rightarrow \left(\begin{array}{cc} \uparrow & \downarrow \\ & \downarrow\uparrow \end{array} \right) \rightarrow \left(\begin{array}{cc} \uparrow & \downarrow \\ \downarrow & \uparrow \end{array} \right), \tag{89}$$

where the symbol $(\cdot)$ indicates the spin configuration of the f and conduction electrons at the sites i and j:

$$\left(\begin{array}{cc} f_i & f_j \\ s_i & s_j \end{array} \right) \quad (f_i, s_i = |0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\downarrow\uparrow\rangle). \tag{90}$$

In the process above, the local state $|1,1\rangle_i|1,-1\rangle_j$ is transformed to $|1,0\rangle_i|1,0\rangle_j$ where $|\ell = 1, m\rangle_i$ indicates a local triplet at site i with $s_i^z = m$. Similarly other interactions are included and thus the effective Hamiltonian is given by a spin-1 Heisenberg model.

We can generalize the Kondo lattice by including the intersite RKKY interactions between localized spins. Let us investigate the Hamiltonian given by

$$\begin{aligned} H &= \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{ci\uparrow} n_{ci\downarrow} \\ &+ J \sum_i \mathbf{S}_i \cdot \sigma_i + \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \end{aligned} \tag{91}$$

If the lattice is bipartite with respect to $\{J_{ij}\}$, the uniqueness of the ground state is proved in a same manner:

Theorem 2.9 We investigate the Kondo lattice in eq.(91) at half filling. Let us assume that the lattice Λ is bipartite and connected with respect to $\{t_{ij}\}$. We further assume that Λ is bipartite with respect to $\{J_{ij}\}$ and $J_{ij} \geq 0$. Then the coefficient matrix of the ground state is positive semidefinite for $U > 0$ and $J \neq 0$ at half filling (after a partial electron-hole transformation). Thus the ground state is unique.

This statement indicates that the ground state is continuous with respect to J_{ij} as long as J_{ij} are antiferromagnetic. Probably we don't need to say that we can extend *Theorem 2.7-2.9* to the Hamiltonian where U and J are site dependent.

2.6. *The Kondo-Hubbard model*

Let us consider generalized models which may be called the Kondo-Hubbard model including the Kondo lattice and the two-impurity Kondo model as special cases. The Hamiltonian is written as

$$\begin{aligned} H &= -\sum_{ij\in\Lambda,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\in\Lambda} n_{ci\sigma} + U \sum_{i\in\Lambda} n_{ci\uparrow} n_{ci\downarrow} + J \sum_{i\in\Lambda_f} \mathbf{S}_i \cdot \sigma_i \\ &+ \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \end{aligned} \tag{92}$$

where Λ denotes a lattice of the conduction electrons and Λ_f is a set of sites on which the localized spins are located. $n_{ci\sigma}$ indicate number operators: $n_{ci\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. We investigate the case where Λ_f is a subset of Λ: $\Lambda_f \subset \Lambda$. Let us assume that Λ is bipartite and divided into two sublattices A and B. We denote the numbers of sites in A and B sublattices of Λ as N_A and N_B, and those in Λ_f as L_A and L_B, respectively: $N_A + N_B = |\Lambda|$ and $L_A + L_B = |\Lambda_f|$ ($N_A \geq L_A$, $N_B \geq L_B$). For the Kondo lattice, we have $N_A = L_A$ and $N_B = L_B$. A similar argument in the section **2.5** proves the uniqueness of the ground state.

Theorem 2.10 Let us consider the Kondo-Hubbard model on a connected and bipartite lattice in eq.(92) at half filling. We assume that the lattice is bipartite with respect to $\{J_{ij} \geq 0\}$. Then the ground state is unique for $U > 0$ and $J \neq 0$ (apart from a trivial degeneracy with respect to S^z for $J < 0$). The total spin is given by

$$S = |N_A - N_B - L_A + L_B|/2 \quad \text{for} \quad J > 0,$$
$$S = |N_A - N_B + L_A - L_B|/2 \quad \text{for} \quad J < 0.$$

Since a proof of the uniqueness is very similar to that for the Kondo lattice, we don't repeat it here. The total spin of the ground state for $J > 0$ is given by the *Lemma 2.3* for the spin-1/2 Heisenberg model. For the ferromagnetic exchange interaction $J < 0$, one can determine S employing the Perron-Frobenius theorem, which will be discussed in the Chapter **3**. For the Kondo lattice, $S = 0$ for $J > 0$ and $S = |N_A - N_B|$ for $J < 0$.

As a corollary, we show a statement about the two-impurity Kondo model, for which there has been a debate about a singular fixed point found in the numerical renormalization group method.[77] The Hamiltonian is written in the form:

$$\begin{aligned} H &= \sum_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{ci\uparrow} n_{ci\downarrow} \\ &+ J \sum_{j=1,2} \mathbf{S}_j \cdot \sigma_j + J_{RK} \mathbf{S}_1 \cdot \mathbf{S}_2. \end{aligned} \tag{93}$$

Corollary Let us assume that the lattice is bipartite and connected and $J_{RK} \geq 0$ for $1 \in A$ and $2 \in B$ (or $1 \in B$ and $2 \in A$) or $J_{RK} \leq 0$ for $1, 2 \in A$ (or $1, 2 \in B$). Then the ground state of the two-impurity Kondo model at half filling for $U > 0$ and $J \neq 0$ is unique and continuous with respect to $J(\neq 0)$. Thus the ground state has no singularity as a function of $J(\neq 0)$ on a finite lattice.

This is a direct consequense of *Theorem 2.10* and consistent with the results by Monte Carlo simulations,[78] numerical renormalization group calculations[79] and diagonalizations.[80] We can expect a sharp crossover between the on-site Kondo region and the RKKY region; in the former case we have a local singlet at each site and in the latter case localized spins are in a collective state.

As an example of the Theorem, we point out that the ferromagnetism of the poly(m-phenylenecarbene) is explained by the Kondo-Hubbard model with ferromagnetic exchange term $J < 0$.[85,87] This organic material contains carbon sites called carbene, where a non-bonding localized electron couples with a π electron on the bridge through the Hund's coupling.[87]

2.7. *Inequalities for correlation functions*

The spin-reflection positivity for the half-filled band with the repulsive Coulomb interactions is closely related with antiferromagnetic correlations between the conduction electrons (and the localized spins). If C is positive definite, we can show

$$TrC^{\dagger}MCM^{\dagger} > 0, \tag{94}$$

for a square matrix M. This inequality is easily derived as follows. Let ϵ_{α} and $|\alpha\rangle$ be eigenvalues and corresponding eigenvectors : $C|\alpha\rangle = \epsilon_{\alpha}|\alpha\rangle$. Then $TrC^{\dagger}MCM^{\dagger} = \sum_{\alpha\beta}\epsilon_{\alpha}\epsilon_{\beta}|\langle\alpha|M|\beta\rangle|^2 > 0$.

By virtue of the property in eq.(94), one can derive inequalities for correlation functions. If we take $M^{\sigma}_{\alpha\alpha'} = \langle\psi^{\sigma}_{\alpha}|n_{ci\sigma}|\psi^{\sigma}_{\alpha'}\rangle$, we obtain a trivial inequality:

$$TrC^{\dagger}M^{\uparrow}CM^{\downarrow\dagger} = \langle n_{ci\uparrow}n_{ci\downarrow}\rangle_{\tilde{H}} = \langle n_{ci\uparrow}(1-n_{ci\downarrow})\rangle_H > 0, \tag{95}$$

where $\langle\cdot\rangle_H$ and $\langle\cdot\rangle_{\tilde{H}}$ denote the expectation values in the original and transformed space, respectively. For the choice $M^{\sigma}_{\alpha\alpha'} = \langle\psi^{\sigma}_{\alpha}|n_{ci\sigma}-n_{cj\sigma}|\psi^{\sigma}_{\alpha'}\rangle$, we have $0 < \langle(n_{ci\uparrow}-n_{cj\uparrow})(n_{ci\downarrow}-n_{cj\downarrow})\rangle_{\tilde{H}} = -\langle(n_{ci\uparrow}-n_{cj\uparrow})(n_{ci\downarrow}-n_{cj\downarrow})\rangle_H$, i.e.

$$\langle n_{ci\uparrow}n_{ci\downarrow}+n_{cj\uparrow}n_{cj\downarrow}\rangle_H \ < \ \langle n_{ci\uparrow}n_{cj\downarrow}+n_{ci\downarrow}n_{cj\uparrow}\rangle_H \quad (i\neq j). \tag{96}$$

Similarly we can show $-1/4 < \ \langle S^z_i S^z_j\rangle_H \ < 1/4$ for $S^z_i = n_{fi\uparrow}-n_{fi\downarrow}$ or $n_{ci\uparrow}-n_{ci\downarrow}$.

We can obtain non-trivial inequalities when we choose $M^{\sigma} = \langle c^{\dagger}_{i\sigma}c_{j\sigma}\rangle$, $\langle f^{\dagger}_{i\sigma}f_{j\sigma}\rangle$ or $\langle c^{\dagger}_{i\sigma}f_{i\sigma}\rangle$, which corresponds to consider correlation functions defined by

$$S_{ff}(i,j) = \langle S^{+}_i S^{-}_j\rangle, \tag{97}$$

$$S_{cc}(i,j) = \langle\sigma^{+}_i\sigma^{-}_j\rangle, \tag{98}$$

and

$$S_{fc}(i) = \langle S^{+}_i\sigma^{-}_i\rangle, \tag{99}$$

where spin operators are $S^{+}_i = f^{\dagger}_{i\uparrow}f_{i\downarrow}$, $\sigma^{+}_i = c^{\dagger}_{i\uparrow}c_{i\downarrow}$, $S^{-}_i = (S^{+}_i)^{\dagger}$ and $\sigma^{-}_i = (\sigma^{+}_i)^{\dagger}$.

For the Hubbard model with $U > 0$ at half filling, we can show by making the electron-hole transformation for $i \in A$ and $j \in B$,

$$\begin{aligned} S_{cc}(i,j) &= \langle c^{\dagger}_{i\uparrow}c_{i\downarrow}c^{\dagger}_{j\downarrow}c_{j\uparrow}\rangle_H = -\langle c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow}c_{j\downarrow}c_{j\uparrow}\rangle_{\tilde{H}} \\ &= -TrC^{\dagger}K^{\uparrow}_{ij}C(K^{\downarrow}_{ij})^{\dagger} < 0, \end{aligned} \tag{100}$$

where the second equality is due to the electron-hole transformation and we have defined

$$(K^{\sigma}_{ij})_{\alpha\alpha'} = \langle\psi^{\sigma}_{\alpha}|c^{\dagger}_{i\sigma}c_{j\sigma}|\psi^{\sigma}_{\alpha'}\rangle. \tag{101}$$

Similarly we obtain

$$S_{cc}(i,j) > 0 \quad for \quad i,j \in A \quad or \quad i,j \in B. \tag{102}$$

For the Kondo lattice at half filling, it is easy to prove the following.[84]

$$S_{ff}(i,j) < 0; \quad i \in A, j \in B, \tag{103}$$

$$S_{cc}(i,j) < 0; \quad i \in A, j \in B, \tag{104}$$

$$S_{ff}(i,j) > 0; \quad i \in A, j \in A, \tag{105}$$

$$S_{cc}(i,j) > 0; \quad i \in A, j \in A. \tag{106}$$

For the on-site c-f correlations, we can show

$$S_{fc}(i) < 0 \quad for \quad J > 0, \tag{107}$$

$$S_{fc}(i) > 0 \quad for \quad J < 0. \tag{108}$$

Note that we have chosen the different signs for f electrons in the electron-hole transformation for $J < 0$. The equations above indicates that the nearest-neighbor spins are in an antiferromagnetic order and that the RKKY interactions are oscillating functions of the distance between two localized spins.

We can obtain stronger inequalities for spin-correlation functions.[88] Let us note

$$\langle (1 - xc^\dagger_{i\uparrow} c_{j\uparrow})(1 - xc^\dagger_{i\downarrow} c_{j\downarrow}) \rangle_{\tilde{H}} = TrC^\dagger L^\uparrow_{ij} C L^{\downarrow\dagger}_{ij} > 0, \tag{109}$$

for real x and $(L^\sigma_{ij})_{\alpha\alpha'} = \delta_{\alpha\alpha'} - x(K^\sigma_{ij})_{\alpha\alpha'}$. For $i \in A$ and $j \in B$, the above inequality indicates the following after the electron-hole transformation for down-spin electrons,

$$1 - x\langle c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{j\downarrow} c_{i\downarrow} \rangle_H - x^2 l \langle \sigma^+_i \sigma^-_j \rangle_H \ > 0. \tag{110}$$

Since this holds for any real x, we have the correlation inequality

$$\langle \sigma^+_i \sigma^-_j \rangle_H \ < \ -\frac{1}{4}(\langle c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{j\downarrow} c_{i\downarrow} \rangle_H)^2 = -(\langle c^\dagger_{i\uparrow} c_{j\uparrow} \rangle_H)^2, \tag{111}$$

for $U > 0$. Note that for the non-interacting Hubbard model, the equality holds:

$$\langle \sigma^+_i \sigma^-_j \rangle_H = -\frac{1}{4}(\langle c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{j\downarrow} c_{i\downarrow} \rangle_H)^2 \quad (U = 0). \tag{112}$$

The inequality in eq.(111) is stronger than eq.(104). For $i,j \in A$ or $i,j \in B$, we have

$$\langle \sigma^+_i \sigma^-_j \rangle_H \ > \ \frac{1}{4}(\langle c^\dagger_{i\uparrow} c_{j\uparrow} - c^\dagger_{j\downarrow} c_{i\downarrow} \rangle_H)^2, \tag{113}$$

which is, however, equivalent to eq.(102) because of the up-down symmetry. A family of the correlation inequalities is followed straightforwardly according to the reflection positivity in the spin space.

2.8. *η-spin operators*

In this section let us summarize about η-spin operators which were considered deeply by Yang and Zhang.[89,90] The η-spin operators are defined by

$$\eta^\dagger = \sum_j \epsilon_j c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \equiv J^+, \tag{114}$$

$$\eta = \sum_j \epsilon_j c_{j\downarrow} c_{j\uparrow} \equiv J^-, \tag{115}$$

$$J^z = \frac{1}{2}\sum_j (c_{j\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{j\downarrow} - 1), \tag{116}$$

where ϵ_j is given by $\epsilon_j = 1$ if $j \in A$ and $\epsilon_j = -1$ if $j \in B$. The η-spin operators are obtained from the ususal spin operators by the partial electron-hole transformation. We have assumed that the lattice is divided into two subsets A and B. The commutation relations are given as

$$[J^+, J^-] = 2J^z, \tag{117}$$

$$[J^+, J^z] = -J^+; \quad [J^-, J^z] = J^-. \tag{118}$$

In this section, let us consider the Hubbard model:

$$H = -t\sum_{\langle ij\rangle} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow}. \tag{119}$$

One can obtain easily

$$[H, J^+] = (U - 2\mu)J^+, \tag{120}$$

$$[H, J^-] = -(U - 2\mu)J^-, \tag{121}$$

$$[H, J^z] = [H, \mathbf{J}^2] = 0, \tag{122}$$

where $\mathbf{J}^2 = (1/2)(J^+J^- + J^-J^+) + (J^z)^2$. Thus the Hubbard model has two $SU(2)$ symmetries, which means the true $SU(2)$ symmetry and the η-spin $SU(2)$ symmetry. We can diagonalize $\mathbf{S}^2$, S^z, $\mathbf{J}^2$, J^z and H simultaneously. Since

$$S^z + J^z = \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} - 1) = integer, \tag{123}$$

the Hamiltonian has $SO(4) = SU(2) \otimes SU(2)/\mathbf{Z}_2$ symmetry. Let us denote the magnitude of the total η-spin as J. A pair of the total spins (S, J) is transformed to (J, S) by the partial electron-hole trnsformation. J is related to the existence of superconductivity, while S is related to the magnetism of the system. The η-operators are sometimes called pseudospin operators.

Let us first investigate the repulsive $U > 0$ case. It can be considered that in one dimension the ground state of the Bethe ansatz solution[13] has the lowest value of the η-spin for the repulsive Hubbard model.[92] We may expect that the ground state is in

the subspace of lowest weight of η-spin even for two or three dimensions. Let N_e be the number of electrons. The z-component of the total η-spin has $J^z = \frac{1}{2}(N_e - |\Lambda|)$. Thus we have $J \geq |N_e - |\Lambda||/2$. We can show that $J = 0$ for the half-filled band because of the positive definiteness of the ground state.

Theorem 2.11 We consider the Hubbard model on a bipartite and connected lattice at half filling. Then the ground state has $J = 0$ for $U > 0$.

Proof By the electron-hole transformation for the up-spin electrons, the Hamiltonian is mapped to the negative-U Hubbard model with an even number of electrons. The ground state of the transformed Hamiltonian is unique and has $S = 0$, which indicates that we have $J = 0$ in the original system. □

For the negative-U Coulomb interaction, the ground state can be a superconducting state with enhanced on-site pairing correlations. Yang considered a variational function given as

$$\psi_\eta = A(\eta^\dagger)^{N_e/2}|0\rangle, \tag{124}$$

where A is a normalization constant and N_e is the number of electrons. He called ψ_η the η-paring state. It is easy to see that ψ_η is an eigenstate of the Hamiltonian:

$$H\psi_\eta = N_e(U/2 - \mu)\psi_\eta. \tag{125}$$

Here let us consider a question whether the η-paring state can be a ground state or not.

Theorem 2.12 Let us consider the negative-U Hubbard model on a bipartite and connected lattice. We assume that the number of electrons N_e is even and $N_e \leq |\Lambda|$. Then the η-pairing state ψ_η is not a ground state.

Proof By the electron-hole transformation for the up spins, the Hamiltonian is transformed to the positive-U Hubbard model at half filling. In the new system one has $S^z = (|\Lambda| - N_e)/2$, while one has $S^z = 0$ in the original system. In the subspace with $S^z = (|\Lambda| - N_e)/2$, the lowest-energy state is unique and the total spin is given by *Lemma 2.3* following an argument of Lieb and Mattis:[57]

$$S = Max\{(|\Lambda| - N_e)/2, ||A| - |B||/2\}, \tag{126}$$

where $Max\{X, Y\}$ indicates larger one in X and Y. Hence in the original system the total spin of η-operators is given by

$$J = Max\{(|\Lambda| - N_e)/2, ||A| - |B||/2\}. \tag{127}$$

On the other hand, it is followed from direct calculations that the η-paring state ψ_η has $J = |\Lambda|/2$,[89] or

$$\mathbf{J}^2\psi_\eta = \frac{|\Lambda|}{2}(\frac{|\Lambda|}{2} + 1)\psi_\eta. \tag{128}$$

Therefore the total η-spin of ψ_η is different from that of the true ground state. ψ_η is orthogonal to the ground state. □

From the proof of this theorem, we can say the following.

Corollary For the negative-U Huabbrd model on a bipartite and connected lattice for an even number of electrons, if

$$||\Lambda| - N_e| < ||A| - |B||, \tag{129}$$

then there is off-diagonal long-range order (ODLRO).[91]

Proof This is a direct consequence of the proof of *Theorem 2.12* and the next theorem by Yang and Zhang.[90]

Theorem 2.13 For any state ψ for which $J^2 - (J^z)^2 = O(|\Lambda|)$, there is ODLRO.

We should define ODLRO before a proof of *Theorem 2.13*. Let us define the two-particle density matrix given as:[91,93]

$$\Gamma(r_1' r_2' | r_1 r_2) = \langle \psi | a_{r_1'} a_{r_2'} a_{r_2}^\dagger a_{r_1}^\dagger | \psi \rangle, \tag{130}$$

for a wave function ψ, where a_r are operators for electrons. The coordinate numbers r_i may include spins. If there is a long-range order for ψ, the two-particle density matrix may have large values, for instance, if r_1 is close to r_2 and at the same time r_1' is also close to r_2'. This type of correlation was called an off-diagonal long-range order (ODLRO) by Yang. Here we define ODLRO in the following way.

Definition We define three matrices from the two-partice density matrix Γ:

$$X_{ij} = \Gamma(i\sigma_i, j\sigma_j | i\sigma_i', j\sigma_j'), \tag{131}$$

$$Y_{ij} = \Gamma(i\sigma_i, j\sigma_j | j\sigma_j', i\sigma_i'), \tag{132}$$

$$Z_{ij} = \Gamma(i\sigma_i, i\sigma_i' | j\sigma_j, j\sigma_j'). \tag{133}$$

If one of matrices X, Y and Z has an eigenvalue of the order of the system size $|\Lambda|$, we say that ψ has ODLRO.

Proof of Theorem 2.13 Let us define the matrix Z as

$$Z_{ij} = \langle \psi | c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow} | \psi \rangle. \tag{134}$$

Let λ_2 be the largest eigenvalue of Z. It is clear from the variational principle that

$$\lambda_2 \geq (v, Zv), \tag{135}$$

for any normalized vector v where $(,)$ indicates an inner product. Let us take $v = (v_i)$ as $v_i = \epsilon_i/|\Lambda|^{1/2}$. Then

$$\begin{aligned} \lambda_2 &\geq \langle\psi|\eta^\dagger\eta|\psi\rangle/|\Lambda| \\ &= \langle\psi|J^+J^-|\psi\rangle/|\Lambda| = (J^2 - (J^z)^2 + J + J^z)/|\Lambda| \\ &= \frac{1}{|\Lambda|}(J^2 - (J^z)^2) + O(1) = O(|\Lambda|) \geq 0. \end{aligned} \tag{136}$$

Hence ψ has ODLRO from the definition. □

The η-paring state has ODLRO because $J = |\Lambda|/2$ and $J^z = ||\Lambda| - N_e|/2$. For the square lattice with $|A| = |B|$, ODLRO is not proved by this method since $J = J^z = ||\Lambda| - N_e|/2$.[94] Note that this does not imply an absence of ODLRO.

3. The Perron-Frobenius theorem in Linear algebra

3.1. *Perron-Frobenius theorem: Irreducible case*

The Perron-Frobenius theorem concerns real matrices with non-positive (or non-negative) elements.[98] Such matrices have important applications in the theory of correlated electrons as well as in the theory of probability and economics.[99] First, Perron proved a theorem on the spectra of positive matrices. Second, Frobenius generalized Perron's theorem to irreducible non-negative matrices, where a positive matrix is a special case of an irreducible non-negative matrix. Let us begin with the definitions of a reducible matrix and an irreducible matrix.

Definition A square matrix $A = (a_{ij})$ $(i = 1, 2, \cdots, n; j = 1, 2, \cdots, n)$ is called reducible if there is a permutation which puts it into the form

$$\begin{bmatrix} B & 0 \\ C & D \end{bmatrix} \tag{137}$$

where B and D are square matrices. Otherwise A is called irreducible.

A permutation of a square matrix $A = (a_{ij})$ means a permutation of the rows of A combined with the same permutation of the columns. Let us suppose that $A = (a_{ij})$ corresponds to a linear operator in an n-dimensional vector space with the bases $e_1, \cdots, e_n$. A permutation of A means a renumbering of the basis vectors: a new basis system is given by $e'_1 = e_{\sigma(1)}, e'_2 = e_{\sigma(2)}, \cdots, e'_n = e_{\sigma(n)}$, where $(\sigma(1), \cdots, \sigma(n))$ is a permutation of indices $1, 2, \cdots, n$. Let $B = (b_{ij})$ and $C = (c_{ij})$ be real rectangular matrices of the same dimensions $m \times n$. We write

$$B \geq C \tag{138}$$

if and ony if

$$b_{ij} \geq c_{ij} (i = 1, \cdots, m; j = 1, \cdots, n). \tag{139}$$

We will write

$$B > C \tag{140}$$

if the equality sign can be omitted in all the inequalities.

Definition A rectangular matrix A with real elements $A = (a_{ij})$ is called non-negative $(A \geq 0)$ or positive $(A > 0)$ if all the elements of A are non-negative $(a_{ij} \geq 0)$ or positive $(a_{ij} > 0)$.

Let $\lambda_1, \cdots, \lambda_n$ be eigenvalues of A and we define

$$\rho(A) = Max\{|\lambda_1|, \cdots, |\lambda_n|\}. \tag{141}$$

Now let us investigate the spectral properties of irreducible non-negative matrices.

Theorem 3.1 (Frobenius) Let $A = (a_{ij})$ $(i, j = 1, \cdots, n)$ be an irreducible non-negative square matrix. Then
(a) $\rho(A) > 0$ and $r = \rho(A)$ is an eigenvalue of A. To the eigenvalue r there corresponds an eigenvector $\mathbf{x}$ with positive coordinates:

$$A\mathbf{x} = r\mathbf{x}, \quad \mathbf{x} > 0, \quad \mathbf{x} \in \mathbf{R}^n. \tag{142}$$

(b) If $A \geq B \geq 0$, then for any eigenvalue β of B we have

$$r = \rho(A) \geq |\beta|. \tag{143}$$

If B has eigenvalue β such that $r = |\beta|$, then $A = B$. (c) $r = \rho(A)$ is a simple eigenvalue, i.e. r is a simple root of the secular equation $det(xI - A) = 0$, where I is a unit matrix.

In the following we call $r = \rho(A)$ the Frobenius eigenvalue of A. If we multiply A by (-1), we can make all the coordinates negative and we can discuss the lowest eigenvalue. The diagonal elements are not important in an application to the Hamiltonian H since we can add a constant matrix cI to H (where c is a real constant). We will show a proof of *Theorem 3.1* in the next section. As a special case, the Perron's theorem is derived where the matrix A is positive $(A > 0)$. It is convention that we call *Theorem 3.1* the Perron-Frobenius theorem. We present some important porperties of the Frobenius eigenvalue below.

Theorem 3.2 Let A be an irreducible non-negative square matrix. Let us assume that $\alpha \in \mathbf{R}, x \in \mathbf{R}^n, \alpha \geq 0, \mathbf{x} \geq 0$, and $\mathbf{x} \neq 0$. If $A\mathbf{x} = \alpha\mathbf{x}$, then $\alpha = \rho(A)$ and $\mathbf{x} > 0$.

Theorem 3.3 For an irreducible non-negative square $n \times n$ matrix A and $\mathbf{x} \in \mathbf{R}^n$ $(\mathbf{x} \geq 0, \mathbf{x} \neq 0)$, we set $A\mathbf{x} = \mathbf{y}$. We define

$$\alpha_A(\mathbf{x}) = Min\{\frac{y_i}{x_i}\}, \quad \beta_A(\mathbf{x}) = Max\{\frac{y_i}{x_i}\}, \tag{144}$$

where we exclude the values of i for which $x_i = 0$. Then

$$\alpha_A(\mathbf{x}) \leq \rho(A) \leq \beta_A(\mathbf{x}). \tag{145}$$

If $\alpha_A(\mathbf{x}) < \rho(A) < \beta_A(\mathbf{x})$, then

$$\alpha_A(\mathbf{x}) < \rho(A) < \beta_A(\mathbf{x}). \tag{146}$$

Theorem 3.4 For an irreducible non-negative square $n \times n$ matrix A, we let $B = 1 + A$. Let

$$\mathbf{a}_j = B^j\mathbf{a} \quad (j = 1, 2, \cdots), \tag{147}$$

for $\mathbf{a} > 0$, $\mathbf{a} \in \mathbf{R}^n$. Then we have

$$\alpha_B(\mathbf{a}_1) \leq \alpha_B(\mathbf{a}_2) \leq \cdots, \tag{148}$$

$$\beta_B(\mathbf{a}_1) \geq \beta_B(\mathbf{a}_2) \geq \cdots, \tag{149}$$

and

$$\lim_{j\to\infty} \alpha_B(\mathbf{a}_j) = \lim_{j\to\infty} \beta_B(\mathbf{a}_j) = 1 + \rho(A). \tag{150}$$

($\alpha_B(\mathbf{a}_j)$ and $\beta_B(\mathbf{a}_j)$ are defined in *Theorem 3.3.*)

These theorems tells us a method to obtain the maximal eigenvalue and a corresponding eigenvector with positive coordinates for an irreducible non-negative square matrix. Let us show several examples.

Example 1 Let H to be

$$H = \begin{bmatrix} 0 & -1 & 0 & -1 \\ -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & -1 \\ -1 & 0 & -1 & 0 \end{bmatrix} \tag{151}$$

which is the Hamiltonian for a fermion on a 4-site lattice. Let $A = -H$. We set $a_1 = (1, 1, 1, 1)^t$. Then $a_2 = Aa_1 = (2, 2, 2, 2)^t$ and we have $\alpha_A(a_1) = \beta_A(a_1) = 2$, i.e. $r = 2$. Hence the lowest eigenvalue of H is -2.

Example 2 A second example is less trivial, which is given by

$$H = \begin{bmatrix} 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & -1 \\ -1 & -1 & U & 0 \\ -1 & -1 & 0 & U \end{bmatrix}. \tag{152}$$

This is the Hamiltonian for the 2-site and 2-electron model where basis states are given as $\psi_1 = -c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}|0\rangle$, $\psi_2 = c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}|0\rangle$, $\psi_3 = c^\dagger_{1\downarrow}c^\dagger_{1\uparrow}|0\rangle$, and $\psi_4 = c^\dagger_{2\downarrow}c^\dagger_{2\uparrow}|0\rangle$. For example, we set $U = 2$ and define $A = -H + 2I$. Let us start from a vector $a_1 = (1, 1, 1, 1)^t$. Then one can easily obtain (we normalize vectors in which the last component equals 1.0),

$$a_2 = Aa_1/2 = (2, 2, 1, 1)^t, \quad \alpha(a_1) = 2, \beta(a_1) = 4, \tag{153}$$

$$\cdots \tag{154}$$

$$a_6 = (1.625, 1.625, 1, 1)^t, \quad \alpha(a_5) = 3.2, \beta(a_5) = 3.25, \tag{155}$$

$$\cdots \tag{156}$$

$$a_{11} = (1.61798, 1.61798, 1, 1)^t, \quad \alpha(a_{10}) = 3.2359550, \beta(a_{10}) = 3.2363636. \tag{157}$$

Thus we have $3.2359550 \leq r \leq 3.2363636$. This implies that the ground-state energy of $H = -A + 2I$ is given as $-1.2359550 \leq E_g \leq -1.2363636$. The exact value is $E_g = -1.2360680$ and the eigenvector is $v = ((1+\sqrt{5})/2, (1+\sqrt{5})/2, 1, 1)^t = (1.61803, 1.61803, 1, 1)^t$. For the general $U > 0$, we can proceed with the same method. Let $a_n = (1, 1, x_n, x_n)^t$ $(0 < x_n < 1)$. Then

$$Aa_n = \begin{bmatrix} U + 2x_n \\ U + 2x_n \\ 2 \\ 2 \end{bmatrix}, \quad \alpha(a_n) = U + 2x_n, \beta(a_n) = 2/x_n. \tag{158}$$

(Here we have assumed that $U + 2x_n \leq 2/x_n$.) In the limit $n \to \infty$, we have $U + 2x = 2/x$ for $x = \lim x_n$. Then the lowest eigenvalue of H is given by

$$E_g = -2x = \frac{U}{2} - ((\frac{U}{2})^2 + 4)^{1/2}. \tag{159}$$

Next we show an interesting theorem regarding an irreducible non-negative matrix. Let $r = \rho(A)$ be a Frobenius eigenvalue of A. We have two cases:
(I) $r > |\alpha|$ for any other eigenvalue $\alpha(\neq r)$ of A. In this case we say that A is primitive.
(II) There are eigenvalues $\lambda_1, \cdots, \lambda_k$ for which $r = |\lambda_i|$ $(i = 1, \cdots, k, k \geq 2)$. In this case A is said to be imprimitive.
For an imprimitive matrix A, A has a structure mentioned below.

Theorem 3.5 (Frobenius) Let A be an irreducible non-negative $n \times n$ matrix. We assume that there are k eigenvalues λ_i $(i = 1, \cdots, k)$ $(k \geq 2)$ where the absolute values are equal to the Frobenius eigenvalue. Then (a) λ_i $(i = 1, \cdots, k)$ is simple root of the secular equation of A, and we can write

$$\lambda_{n+1} = \rho(A) e^{i2\pi n/k}, \quad n = 0, 1, \cdots, k-1. \tag{160}$$

(b) By a permutation matrix P, A is written as

$$P^{-1}AP = \begin{bmatrix} 0 & A_{12} & 0 & \dots & 0 \\ 0 & 0 & A_{23} & \dots & 0 \\ \dots & & & \dots & \\ A_{k1} & 0 & 0 & \dots & 0 \end{bmatrix}. \tag{161}$$

For a primitive matrix A, we can say about an existence of limit A^m. The behavior of A^m in the limit $m \to \infty$ is crucially dependent on whether A is primitive or not.

Theorem 3.6 Let $A \geq 0$ an irreducible square matrix. Then if and only if $\rho(A) = 1$ and A is primitive, we have

$$\lim_{n \to \infty} A^n = A^* \neq 0. \tag{162}$$

3.2. *Perron-Frobenius theorem: General case*

Now let us go over to reducible matrices. Some properties of irreducible non-negative matrices are preserved for reducible ones, since a reducible matrix is obtained as the limit of a sequence of irreducible matrices.

Theorem 3.7 Let A be a non-negative $n \times n$ matrix.
(a) A has a non-negative eigenvalue r. To this eigenvalue r there corresponds a non-negative eigenvector:

$$Ax = rx \quad (x \geq 0,\ x \neq 0). \tag{163}$$

(b) The absolute value of all the eigenvalues of A do not exceed r.

This theorem is also sometimes called the Perron-Frobenius theorem. We again call r as the Frobenius eigenvalue. A uniqueness of the eigenvector with the maximal eigenvalue is not guaranteed because A may be reduced to a triangular block form. In the next section we show a proof. Instead, a short proof for *Theorem 3.7* (a) is presented here by virtue of Brouwer fixed point theorem.

Proof of (a) We can assume that every column of A has at least one non-zero element. (Otherwise 0 is an eigenvalue and the theorem holds.) Let $N = \{\mathbf{x} | ||\mathbf{x}||^2 = \sum_{i=1}^n x_i^2 = 1, \mathbf{x} \geq 0\}$. We define a continuous mapping $\mathbf{f}(\mathbf{x}) : N \to N$ by

$$\mathbf{f}(\mathbf{x}) = \frac{1}{||A\mathbf{x}||} A\mathbf{x}. \tag{164}$$

Clearly, if $\mathbf{x} \in N$, then $\mathbf{f}(\mathbf{x}) \in N$. Thus it is from the Brouwer theorem (see the Lemma below) that the mapping $\mathbf{f}(\mathbf{x})$ has a fixed point. For some $\mathbf{x}^*$, we have

$$\mathbf{f}(\mathbf{x}^*) = \mathbf{x}^*, \quad \mathbf{x}^* \in N. \tag{165}$$

Hence

$$\frac{1}{||Ax^*||} A\mathbf{x}^* = \mathbf{x}^*. \tag{166}$$

We let $r = ||Ax^*||$, for which $r \geq 0$ since $a_{ij} \geq 0$ and $\mathbf{x}^* \neq 0 (\in N)$. Then we have

$$A\mathbf{x}^* = r\mathbf{x}^*, \tag{167}$$

and (a) holds. □

As a reference, we show the Brouwer theorem.[100,101] Let D^n be n-disk defined as $D^n = \{\mathbf{x} \in \mathbf{R}^n | ||\mathbf{x}||^2 = \sum_{i=1}^n x_i^2 = 1\}$.

Lemma 3.8 (Brouwer) A continuous mapping $f : D^n \to D^n$ has a fixed point: $f(\mathbf{x}) = \mathbf{x}$ for some $\mathbf{x} \in D^n$.

Proof Let us assume that $f(x) \neq x$ for any $x \in D^n$. Then $x - f(x) \neq 0$ for any $x \in D^n$. We define a mapping $g : D^n \to S^{n-1}$ as follows. For each $x \in D^n$, $g(x)$

is a projection of x onto S^{n-1} where $x - f(x)$ is parallel to $g(x) - x$. Then $g(x)$ is continuous and $g|S^{n-1}$ is an identity mapping. However, this mapping is impossible because D^n and S^{n-1} have different topological invariants,[100]

$$H_{n-1}(D^n) = 0, \quad H_{n-1}(S^{n-1}) = \mathbf{Z}. \tag{168}$$

Hence f has a fixed point. □

Lastly we show one statement for a non-negative matrix.

Theorem 3.9 Let A be a $n \times n$ non-negative matrix and r be the Frobenius eigenvalue of A. For $\mathbf{x} = (x_1, \cdots, x_n) > 0$, we set

$$\lambda_x = \min_{1 \le i \le n} \frac{\sum_{j=1}^n a_{ij} x_j}{x_i}, \quad \Lambda_x = \max_{1 \le i \le n} \frac{\sum_{j=1}^n a_{ij} x_j}{x_i}. \tag{169}$$

Then

$$\lambda_x \le r \le \Lambda_x. \tag{170}$$

If A is irreducible,

$$\max_x \lambda_x = r = \min_x \Lambda_x. \tag{171}$$

Corollary

$$\min_{1 \le i \le n} \sum_{j=1}^n a_{ij} \le r \le \max_{1 \le i \le n} \sum_{j=1}^n a_{ij}, \tag{172}$$

$$\min_{1 \le j \le n} \sum_{i=1}^n a_{ij} \le r \le \max_{1 \le j \le n} \sum_{i=1}^n a_{ij}. \tag{173}$$

3.3. *Appendix: Proof of the Perron-Frobenius theorem*

In this section the Perron-Frobenius theorem is proved, where we follow the treatments in Refs.[102,103]. First let us consider the following Lemmas.

Lemma 3.10 For an $n \times n$ irreducible matrix A,

$$(I + A)^{n-1} > 0, \tag{174}$$

where I is a unit matrix.

Proof Let $A = (a_{ij})$ and $\Gamma = \{(i,j) \in \Omega \times \Omega | a_{ij} \neq 0\}$ for $\Omega = \{1, 2, \cdots, n\}$. We set $A^m = (a_{ij}^{(m)})$. We define $\Gamma(i,j)$ as a set of path connecting i and j, that is, if $\sigma = (i, i_1, \cdots, i_{m-1}, j) \in \Gamma(i,j)$, then $a_{ii_1} \neq 0$, $a_{i_1 i_2} \neq 0, \cdots, a_{i_{m-2} i_{m-1}} \neq 0$ and $a_{i_{m-1} j} \neq 0$. We write $L(\sigma) = m$ which is called the length of σ. Then

$$\begin{aligned} a_{ij}^{(m)} &= \sum_{i_1, \cdots, i_{m-1}} a_{ii_1} a_{i_1 i_2} \cdots a_{i_{m-1} j} \\ &= \sum_{\sigma \in \Gamma(i,j), L(\sigma) = m} a_\sigma, \end{aligned} \tag{175}$$

where $a_\sigma = a_{i_0 i_1} a_{i_1 i_2} \cdots a_{i_{m-1} i_m}$ $(i_0 = i)$. Hence $a_{ij}^{(m)} > 0$ if and only if there exists $\sigma \in \Gamma(i,j)$ such that $a_\sigma > 0$ and $L(\sigma) = m$. One can assume that in $\sigma = (i_0, i_1, \cdots, i_m)$ indices $i_0, i_1, \cdots, i_m$ are different each other. This indicates that if $\Gamma(i,j) \neq \phi$, we have an element $\sigma = (i_0, i_1, \cdots, i_m) \in \Gamma(i,j)$ such that $m+1 \leq |\Omega| = n$, i.e. $m \leq n-1$. Therefore $\Gamma(i,j) \neq \phi$ implies

$$a_{ij} + a_{ij}^{(2)} + \cdots + a_{ij}^{(n-1)} > 0. \tag{176}$$

Since A is irreducible, $\Gamma(i,j) \neq \phi$ for $i \neq j$ and then (i,j) element x_{ij} of $(I+A)^{n-1}$ is positive because of eq.(176):

$$x_{ij} = (n-1)a_{ij} + \begin{pmatrix} n-1 \\ 2 \end{pmatrix} a_{ij}^{(2)} + \cdots + a_{ij}^{(n-1)} > 0. \tag{177}$$

Obviously, the diagonal elements of $(I+A)^{n-1}$ is $\geq 1 > 0$. □

Lemma 3.11 For a non-negative $n \times n$ matrix A and a real positive number s, $\rho(A) < s$ if and ony if there is some $\mathbf{y} > 0$ $(\mathbf{y} \in \mathbf{R}^n)$ such that $s\mathbf{y} > A\mathbf{y}$.

Proof Let us suppose that $\rho(A) < s$. Then $\rho(B) < 1$ for $B = A/s$. Since the absolute value of every eigenvalue of B is less than 1, $I + B + B^2 + \cdots$ converges and equals $(I-B)^{-1}$. Hence $(I-B)^{-1} \geq 0$. Let $\mathbf{z} = (1, \cdots, 1)^t$, then $(I-B)^{-1}\mathbf{z} = \mathbf{y} > 0$. (Note that each row of $(I-B)^{-1}$ has at least one non-zero element.) Since $\mathbf{z} = (I-B)\mathbf{y}$, we have $\mathbf{y} > B\mathbf{y}$.

Inversely, suppose that $\mathbf{y} > B\mathbf{y}$ for $\mathbf{y} > 0$ and $B = A/s$. Let $\mathbf{u} = \mathbf{y} - B\mathbf{y} > 0$, then $B^i\mathbf{u} \geq 0$ $(i = 1, 2, \cdots)$. It is easy to see that

$$\begin{aligned} \mathbf{u}_m &= \mathbf{u} + B\mathbf{u} + B^2\mathbf{u} + \cdots + B^m\mathbf{u} = (I + B + B^2 + \cdots + B^m)(I-B)\mathbf{y} \\ &= \mathbf{y} - B^{m+1}\mathbf{y} \leq \mathbf{y}. \end{aligned} \tag{178}$$

If we write $\mathbf{u}_m = (v_1^{(m)}, \cdots, v_n^{(m)})$, then we obtain a bounded and monotonically increasing sequence: $v_j^{(1)} \leq v_j^{(2)} \leq \cdots$. Since $\mathbf{u}_m$ converges, we have $\mathbf{u}_m - \mathbf{u}_{m-1} \to 0$, i.e. $B^m\mathbf{u} \to 0$. Hence $B^m \to 0$ since $\mathbf{u} > 0$. This indicates that $\rho(B) < 1$. □

Proof of Theorem 3.1 (a) Let $\{s_i\}$ be a sequence such that $s_1 > s_2 > \cdots > r$ and $\lim s_i = r$. It is followed from *Lemma 3.11* that $s_i\mathbf{y}_i > A\mathbf{y}_i$ for some $\mathbf{y}_i > 0$ $(\mathbf{y}_i \in \mathbf{R}^n)$. We can suppose that $||\mathbf{y}_i|| = 1$. Since $\{\mathbf{y}_i\}$ is bounded in $\mathbf{R}^n$, $\{\mathbf{y}_i\}$ (or its subsequence) converges to some limit. Let $\mathbf{y} = \lim \mathbf{y}_i$. Obviously $\mathbf{y} \geq 0$ and $||\mathbf{y}|| = 1$. Since $s_i\mathbf{y}_i > A\mathbf{y}_i$, we have $r\mathbf{y} \geq A\mathbf{y}$.

Now we show that $r\mathbf{y} = A\mathbf{y}$. Since $(I+A)^{n-1} > 0$ from *Lemma 3.10*, we have $\mathbf{v} \equiv (I+A)^{n-1}\mathbf{y} > 0$. Suppose that $r\mathbf{y} \neq A\mathbf{y}$, then

$$0 < (I+A)^{n-1}(rI - A)\mathbf{y} = (rI - A)(I+A)^{n-1}\mathbf{y} = r\mathbf{v} - A\mathbf{v}. \tag{179}$$

Then $r\mathbf{v} > A\mathbf{v}$ is followed. $\mathbf{v} > 0$ indicates that $r > \rho(A)$. This is a contradiction. Hence we have $r\mathbf{y} = A\mathbf{y}$.

Next we show that $\mathbf{y} > 0$ and $r > 0$. The former is followed from $0 < (I + A)^{n-1}\mathbf{y} = (1 + r)^{n-1}\mathbf{y}$. To show the latter, suppose that $r = 0$. Then $A\mathbf{y} = 0$, which leads to $A = 0$ since $\mathbf{y} > 0$. Hence $(I + A)^{n-1} = I$ which contradicts with $(I + A)^{n-1} > 0$.

(b) Let $B = (b_{ij})$. Let β be any eigenvalue of B: $B\mathbf{x} = \beta\mathbf{x}$ ($\mathbf{x} = (x_1, \cdots, x_n)^t \neq 0$). Since $\rho(A^t) = \rho(A)$, there exists $\mathbf{y} > 0$ ($\mathbf{y} \in \mathbf{R}^n$) such that $A^t\mathbf{y} = r\mathbf{y}$ for $r = \rho(A)$. We define $\mathbf{x}^+$ as $\mathbf{x}^+ = (|x_1|, \cdots, |x_n|)^t$. Because $\sum_j b_{ij}x_j = \beta x_i$, we have $\sum_j b_{ij}|x_j| \geq |\beta||x_i|$ or

$$B\mathbf{x}^+ \geq |\beta|\mathbf{x}^+, \quad \mathbf{x} \geq 0. \tag{180}$$

We multiply $\mathbf{y}$ from the left and obtain

$$\beta(\mathbf{y}, \mathbf{x}^+) \leq (\mathbf{y}, B\mathbf{x}^+) \leq (\mathbf{y}, A\mathbf{x}) = r(\mathbf{y}, \mathbf{x}^+). \tag{181}$$

Note that $(\mathbf{y}, \mathbf{x}^+) > 0$ since $\mathbf{y} > 0$ and $\mathbf{x}^+ \geq 0$. Then we have

$$r \geq |\beta|. \tag{182}$$

Let us consider the case where $r = |\beta|$. Then

$$(\mathbf{y}, B\mathbf{x}^+) = (\mathbf{y}, A\mathbf{x}^+) \tag{183}$$

is followed. The fact $\mathbf{y} > 0$ indicates that

$$B\mathbf{x}^+ = A\mathbf{x}^+. \tag{184}$$

Similarly we have $B\mathbf{x}^+ = r\mathbf{x}^+$ from eq.(181). Hence $A\mathbf{x}^+ = r\mathbf{x}^+$. Then it is followed from (a) that $\mathbf{x} > 0$. Thus $A = B$ from eq.(184).

(c) Let $f(t) = det(tI - A)$. Then

$$\begin{aligned} & f'(t) \\ = & \begin{vmatrix} 1 & -a_{12} & \cdots & -a_{1n} \\ 0 & t - a_{22} & \cdots & -a_{2n} \\ \cdots & & & \cdots \\ 0 & -a_{n2} & \cdots & t - a_{nn} \end{vmatrix} + \cdots + \begin{vmatrix} t - a_{11} & -a_{12} & \cdots & 0 \\ -a_{21} & t - a_{22} & \cdots & 0 \\ \cdots & & & \cdots \\ -a_{n1} & -a_{n2} & \cdots & t - a_{nn} \end{vmatrix} \\ = & \ det(tI_{n-1} - A_1) + \cdots + det(tI_{n-1} - A_n), \end{aligned} \tag{185}$$

where I_{n-1} is a unit matrix of degree $n - 1$. Let B_i be a matrix obtained from A by replacing elements in the ith row and ith column by 0. A_i is defined from A by removing ith row and ith column from A. By a permutation matrix P, we can write

$$PB_iP^{-1} = \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & & & \\ \cdots & & A_i & \\ 0 & & & \end{bmatrix}. \tag{186}$$

Hence we have

$$det(tI - B_i) = t \cdot det(tI_{n-1} - A_i). \tag{187}$$

This means that $\rho(B_i) = \rho(A_i)$. Since $A \geq B_i \geq 0$, $\rho(A) \geq \rho(B_i)$ from (b). Thus we have $r = \rho(A) > \rho(B_i) = \rho(A_i)$ $(A \neq B_i)$. This indicates that

$$det(rI_{n-1} - A_i) > 0. \tag{188}$$

Therefore $f'(r) > 0$ and r is a simple root of $f(t) = 0$. □

Proof of Theorem 3.2 Since A^t and A have the same eigenvalues, $\rho(A) = \rho(A^t)$. There exists $\mathbf{y} > 0$ $(\mathbf{y} \in bfR^n)$ such that $A^t\mathbf{y} = r\mathbf{y}$ for $r = \rho(A)$. Then $(\alpha\mathbf{x}, \mathbf{y}) = (A\mathbf{x}, \mathbf{y}) = (\mathbf{x}, A^t\mathbf{y}) = (\mathbf{x}, \alpha\mathbf{y})$. Hence $\alpha(\mathbf{x}, \mathbf{y}) = r(\mathbf{x}, \mathbf{y})$. Since $(\mathbf{x}, \mathbf{y}) > 0$, we have $\alpha = r$. From $(I + A)^{n-1} > 0$, $(I + A)^{n-1}\mathbf{x} = (1 + \alpha)^{n-1}\mathbf{x} > 0$ is followed. Then $\mathbf{x} > 0$. □

Proof of Theorem 3.3 Let $\alpha = \alpha_A(\mathbf{x})$, $\beta = \beta_A(\mathbf{x})$ and $r = \rho(A)$. From the definition, we have $\alpha\mathbf{x} \leq \mathbf{y} = A\mathbf{x} \leq \beta\mathbf{x}$. If we take $\mathbf{z} > 0$ such that $A^t\mathbf{z} = r\mathbf{z}$, then $(\alpha\mathbf{x}, \mathbf{z}) \leq (\mathbf{y}, \mathbf{z}) \leq (\beta\mathbf{x}, \mathbf{z})$. Hence

$$(\alpha\mathbf{x}, \mathbf{z}) \leq (A\mathbf{x}, \mathbf{z}) = (\mathbf{x}, A^t\mathbf{z}) = r(\mathbf{x}, \mathbf{z}) \leq (\beta\mathbf{x}, \mathbf{z}). \tag{189}$$

Since $(\mathbf{x}, \mathbf{z}) > 0$, we have $\alpha \leq r \leq \beta$. If $\alpha = r$, then $\alpha\mathbf{x} = A\mathbf{x}$ is followed from eq.(189) and $\mathbf{z} > 0$. Hence we have $\alpha\mathbf{x} = \mathbf{y}$. It is followed from the definition of α and β that $\beta = \alpha$. Similarly $\beta = r$ implies $\alpha = \beta$. Therefore we have $\alpha < r < \beta$ if $\alpha < \beta$. □

Proof of Theorem 3.4 Let us apply $B \geq 0$ to the inequality $\alpha_B(\mathbf{a}_j)\mathbf{a}_j \leq B\mathbf{a}_j \leq \beta_B(\mathbf{a}_j)\mathbf{a}_j$:

$$\alpha_B(\mathbf{a}_j)\mathbf{a}_{j+1} \leq B\mathbf{a}_{j+1} \leq \beta_B(\mathbf{a}_j)\mathbf{a}_{j+1}. \tag{190}$$

From the definitions of α_B and β_B, we have

$$\alpha_B(\mathbf{a}_j) \leq \alpha_B(\mathbf{a}_{j+1}) \leq \beta_B(\mathbf{a}_{j+1}) \leq \beta_B(\mathbf{a}_j). \tag{191}$$

Since $1 + r = \rho(B)$ $(r = \rho(A))$, we have $\alpha_B(\mathbf{a}_j) \leq 1 + r \leq \beta_B(\mathbf{a}_j)$ $(j = 1, 2, \cdots)$ from *Theorem 3.3*. It is followed from the definition that $I + A$ is primitive. Thus a sequence $\{(B/(1 + r))^j\}_{j=1,2,\cdots}$ has a finite limit $\lim_{j\to\infty}(B/(1 + r))^j$ because of *Theorem 3.6*. Hence for some $\mathbf{b} \in \mathbf{R}^n$,

$$\lim_{j\to\infty}(\frac{B}{1+r})^j\mathbf{a} = \lim_{j\to\infty}(1 + r)^{-j}\mathbf{a}_j = \mathbf{b}. \tag{192}$$

Applying B, we have

$$\lim_{j\to\infty}(1 + r)^{-j}B\mathbf{a}_j = \lim_{j\to\infty}(1 + r)^{-(j+1)}\mathbf{a}_{j+1}(1 + r) = (1 + r)\mathbf{b}. \tag{193}$$

From the definition of α_B and β_B, we obtain

$$\lim_{j\to\infty}\alpha_B(\mathbf{a}_j) = 1 + r, \quad \lim_{j\to\infty}\beta_B(\mathbf{a}_j) = 1 + r. \tag{194}$$

This concludes the proof. □

Proof of Theorem 3.6 Suppose that $\lim_{m\to\infty} A^m = A^* \neq 0$. From a theorem in Linear algebra (see *Lemma 3.12* below), we should have $\rho(A) = 1$ and its multiplicity should be 1. Thus A is primitive.

Inversely, suppose that $\rho(A) = 1$ and A is primitive. Obviously $\lim_{m\to\infty} A^m = A^* \neq 0$ exists from *Lemma 3.12*. □

Lemma 3.12 For a $n \times n$ square matrix A, the following (a) and (b) are equivalent.
(a) There exists a limit $\lim_{n\to\infty} A^n = B$.
(b) For any eigenvalue α of A, we have $|\alpha| < 1$ or $\alpha = 1$. If $\alpha = 1$ is the eigenvalue of A, $\alpha = 1$ is a simple root of the characteristic equation.
(See some text for a proof.)

Proof of Theorem 3.7 (a) Let $A = (a_{ij})$. We define a matrix $A^{(m)} = (a_{ij}^{(m)})$ by $a_{ij}^{(m)} = a_{ij} + 1/m$ for $m = 1, 2, \cdots$. Since $A^{(m)} > 0$, $A^{(m)}$ is irreducible. Then by *Theorem 3.1*, $A^{(m)}$ has the Frobenius eigenvalue $r^{(m)}$ and its corresponding positive eigenvector $\mathbf{x}^{(m)} > 0$:

$$A^{(m)}\mathbf{x}^{(m)} = r^{(m)}\mathbf{x}^{(m)}, \quad r^{(m)} > 0, \quad \mathbf{x}^{(m)} > 0. \tag{195}$$

Let

$$N = \{\mathbf{x} | \sum_{i=1}^{n} x_i = 1, \ \mathbf{x} \geq 0\}. \tag{196}$$

We can assume that $\mathbf{x}^{(m)} \in N$ $(m = 1, 2, \cdots)$. Since N is compact, from $\{\mathbf{x}^{(m)}\}$ we can chose a subsequence

$$\mathbf{x}^{\nu_1}, \mathbf{x}^{\nu_2}, \cdots, \mathbf{x}^{\nu_j}, \cdots, \quad (\nu_1 < \nu_2 < \cdots < \nu_j < \cdots), \tag{197}$$

which converges. Let

$$\mathbf{x} = \lim_{j\to\infty} \mathbf{x}^{\nu_j}. \tag{198}$$

Obviously $A^{(m)} > A^{(m+1)} > A$ $(m = 1, 2, \cdots)$. Then by *Theorem 3.1*(b), we have $r^{(m)} \geq r^{(m+1)} > 0$ $(m = 1, 2, \cdots)$. Thus the sequence $r^{(1)}, r^{(2)}, \cdots, r^{(j)}, \cdots$ is bounded from below and monotonically decreasing, indicating an existence of a limit:

$$r = \lim_{m\to\infty} r^{(m)} \geq 0. \tag{199}$$

Then $\{r^{(\nu_j)}\}$ also converges to r and in the limit $j \to \infty$ we have

$$A\mathbf{x} = r\mathbf{x}. \tag{200}$$

Clearly $\mathbf{x} \geq 0$ since $\mathbf{x} \in N$.

(b) Since $A^{(m)}$ is irreducible and $A^{(m)} > A \geq 0$, we have

$$r^{(m)} \geq |\alpha|, \quad (m = 1, 2, \cdots) \tag{201}$$

for any eigenvalue α of A from *Theorem 3.1*(b). Let $m \to \infty$, then

$$r \geq |\alpha|. \tag{202}$$

Now (b) holds. □

To keep the section within reasonable length, we omit a proof of *Theorem 3.8* since its proof has a little bit large length. See, for example, Ref.[98] for a complete proof.

Proof of Theorem 3.9 Let $\mathbf{y}$ be an eigenvector corresponding to the Frobenius eigenvalue $r = \rho(A^t)$. Then

$$\mathbf{y}^t A = r\mathbf{y}^t, \quad \mathbf{y}^t \geq 0, \tag{203}$$

is followed. From the definition of λ_x and Λ_x, we have

$$\lambda_x x_i \leq \sum_{j=1}^{n} a_{ij} x_j \leq \Lambda_x x_i \quad (i = 1, 2, \cdots, n), \tag{204}$$

and

$$\lambda_x \mathbf{x} \leq A\mathbf{x} \leq \Lambda_x \mathbf{x}. \tag{205}$$

It is followed from eq.(203) that

$$\lambda_x(\mathbf{y}, \mathbf{x}) \leq r(\mathbf{y}, \mathbf{x}) \leq \Lambda_x(\mathbf{y}, \mathbf{x}). \tag{206}$$

Since $(\mathbf{y}, \mathbf{x}) > 0$, we have

$$\lambda_x \leq r \leq \Lambda_x. \tag{207}$$

If A is irreducible, there is a vector $\mathbf{x}^* > 0$ such that $A\mathbf{x}^* = r\mathbf{x}^*$. Therefore

$$r = (\sum_{j=1}^{n} a_{ij} x_j^*)/x_i^*. \tag{208}$$

This implies $r = \lambda_{x^*} = \Lambda_{x^*}$. □

4. Applications of the Perron-Frobenius theorem to interacting systems

4.1. *The Heisenberg model*

Let us discuss the Heisenberg model following the treatment in Refs.[57,104] to prove a uniqueness of the ground state on a finite lattice employing the Perron-Frobenius theorem. We write again the Lemma mentioned in the section **2.4**.

Theorem 4.1 Let us consider the spin-1/2 antiferromagnetic Heisenberg model on a connected and bipartite lattice,

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{209}$$

where $J_{ij} \geq 0$ are non-zero for $i \in A$ and $j \in B$ or $i \in B$ and $j \in A$. Let us denote the number of sites in A and B sublattices as $|A|$ and $|B|$, respectively, and assume that $|A| \geq |B|$. Then the ground state is unique and has $S = (|A| - |B|)/2$.

Proof In the subspace with $S^z = M$, we can choose the basis set $\{\phi_\alpha\}$ where each ϕ_α denote a configuration of spins in the real space. First, let us perform a transformation

$$S_i^x \to -S_i^x, \quad S_i^y \to -S_i^y, \quad S_i^z \to S_i^z \quad (i \in A) \tag{210}$$

and the spins on the B-sublattice are unaltered. The Hamiltonian reads $H = H_0 + H_1$ in the new system, where

$$H_0 = \sum_{ij} J_{ij} S_i^z S_j^z, \tag{211}$$

$$H_1 = -\sum_{ij} J_{ij} \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+). \tag{212}$$

H_1 is the off-diagonal part of H.

Suppose that the z-component S_i^z has $m_i (i \in \Lambda)$ (=1/2 or $-1/2$) in a given state ϕ_α. Then our basis state is given by

$$\phi_\alpha = C (S_1^+)^{\frac{1}{2}+m_1} (S_2^+)^{\frac{1}{2}+m_2} \cdots (S_N^+)^{\frac{1}{2}+m_N} \psi_0, \tag{213}$$

where ψ_0 is the state occupied by down spins at each site and C is a positive normalization constant. Then it is easy to check that the matrix element defined by

$$T_{\beta\alpha} = \langle \phi_\beta | H_1 | \phi_\alpha \rangle \tag{214}$$

is non-positive for any α and β:

$$T_{\beta\alpha} \leq 0. \tag{215}$$

The connectivity of Λ guarantees that $T = (T_{\beta\alpha})$ is irreducible.[a] Hence the Perron-Frobenius theorem implies a uniqueness of the lowest energy state in each subspace

[a] See the section **3.1** for the definition of *irreducible*.

with $S^z = M$. This indicates that the ground state is unique since every energy eigenvalue has a corresponding eigenfunction in the lowest M subspace. The ground state eigenfunction ψ has positive amplitudes for this basis set, i.e.

$$\psi = \sum_\alpha c_\alpha \phi_\alpha, \quad c_\alpha > 0. \tag{216}$$

Now let us consider the total spin of the ground state. If $|A| = |B|$, we can easily construct a trial state with $S = 0$. A simple one is

$$\psi_{tri} = C' \psi_{i_1 j_1} \psi_{i_2 j_2} \cdots \psi_{i_{N/2} j_{N/2}}, \tag{217}$$

where $i_k \in A$, $j_k \in B$ and $C' > 0$. ($i_1, \cdots, i_{N/2}$ are different one another, which also applies to $j_1, \cdots, j_{N/2}$.) $\psi_{i_k j_k}$ denotes a local singlet in which spins are located on sites i_k and j_k. If we compared the signs of amplitudes in the expansion in our basis set $\{\phi_\alpha\}$, we can check that ψ and ψ_{tri} have exactly the same signs (if we go back to the original system). Thus we have $\langle \psi | \psi_{tri} \rangle \neq 0$. Hence ψ has $S = 0$. We can proceed in a similar manner for general cases $|A| > |B|$, where the spins on the different sublattices are in antiferromagnetic-like states and the spins on the same sublattices are ferromagnetic like. □

In the theorem above, the spin of a localized electron is 1/2, but following the original paper[57] we may be extending to deal with various types of localized spins, where the magnitude of spin on each site is s_i. In this case the total spin is given by

$$S = |S_A - S_B|, \tag{218}$$

where S_A and S_B are maximum possible spins on each sublattices,

$$S_A = \sum_{i \in A} s_i, \quad S_B = \sum_{j \in B} s_j. \tag{219}$$

4.2. *Double exchange interaction and ferromagnetism*

In this section let us consider the ferromagnetism induced by double exchange interaction. The double exchange interaction may be important for the ferromagnetism of real materials such as mixed valency compounds. In the subsequent sections we will show several models which exhibit ferromagnetism due to the double exchange interaction. The double exchange interaction was first proposed long time ago by Zener[105] in the study of ferromagnetism of mixed valence compounds such as $La_{1-x}Ca_xMnO_3$. Later Anderson and Hasegawa[106] calculated energy splitting due to the double exchange. In the semiconducting phase each Mn ion has a charge of 3+. When some of the La^{3+} are replaced by Ca^{2+} ions, a corresponding number of Mn^{3+} ions are replaced by Mn^{4+} ions. This doping effect gives rise to electrical conductivity. Let us examine the magnetism of two Mn ions separated by an O^{2-} ion. Following Zener, we assume large Hund couplings so that each Mn ion has its highest multiplicity. We define three configurations as follows.[107]

$$\psi_I : \mathrm{Mn}^{3+}(\uparrow\uparrow)\mathrm{O}^{2-}(\downarrow\uparrow)\mathrm{Mn}^{4+}(\uparrow)$$
$$\psi_{II} : \mathrm{Mn}^{3+}(\uparrow\uparrow)\mathrm{O}^{-}(\downarrow)\mathrm{Mn}^{3+}(\uparrow\uparrow)$$
$$\psi_{III} : \mathrm{Mn}^{4+}(\uparrow)\mathrm{O}^{2-}(\downarrow\uparrow)\mathrm{Mn}^{3+}(\uparrow\uparrow)$$

Since ψ_I and ψ_{III} have the same energy, the ferromagnetic state will be stabilized through the excited state ψ_{II}. This resonance is absent for two Mn ions with antiparallel spins. Hence an effective exchange interaction between Mn^{3+} and Mn^{4+} is ferromagnetic, which is the proposal by Zener called the double exchange.

Let us consider the following process; this may be also called the double exchange where the ferromagnetic couplings between localized spins are induced by succesive exchange interactions between the conduction electrons and the localized spins. We define three states ψ_1, ψ_2 and ψ_3 with $S^z = 1/2$ in which $d_i(\sigma)$ $(i = 1, 2)$ denotes the localized electron with spin σ and the exchange process occurs through the intermediary of $s(\sigma')$ electron.

$$\psi_1 = d_1(\uparrow)s(\downarrow)d_2(\uparrow),$$
$$\psi_2 = d_1(\uparrow)s(\uparrow)d_2(\downarrow),$$
$$\psi_3 = d_1(\downarrow)s(\uparrow)d_2(\uparrow).$$

Suppose that we have an exchange coupling $H = J(\mathbf{S}_1 \cdot \sigma + \mathbf{S}_2 \cdot \sigma)$ between d and s electrons. We have off-diagonal elements of H as

$$\begin{bmatrix} 0 & J/2 & J/2 \\ J/2 & 0 & 0 \\ J/2 & 0 & 0 \end{bmatrix}. \tag{220}$$

Clearly two localized spins are ferromagnetic, which is also seen by the Perron-Fobenius theorem. Maybe we don't need to refer to the Perron-Frobenius theorem for such a small system. For $J < 0$ the ground state has $S = 3/2$ since the eigenvector is positive (> 0). For $J > 0$ the matrix of off-diagonal elements is non-positive for the set of basis $\{-\psi_1, \psi_2, \psi_3\}$ and therefore two localized spins are parallel again.

Based on this consideration, we investigate the Kondo (lattice) Hamiltonian given as

$$H = J \sum_{i\sigma\sigma'} \mathbf{S}_i \cdot c^\dagger_{i\sigma} \sigma_{\sigma\sigma'} c_{i\sigma'} + \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}, \tag{221}$$

where $\mathbf{S}_i$ is the spin-1/2 localized spin on the i-th site and $\sigma_{\sigma\sigma'}$ indicate the Pauli matrices. The localized spins are located on every sites periodically. $c^\dagger_{i\sigma}$ and $c_{i\sigma}$ are operators for the conduction electrons with the transfer matrix elements t_{ij} between the i-th and j-th sites. Here let us assume that $J < 0$ corresponding to the Hund coupling.

Suppose that $|J|$ is large or t_{ij} are small considerably.[108,110] When the transfer term is absent, the eigenstates of H are highly degenerate with respect to spin and

electron configurations. The electron hoppings due to the perturbation produce the double exchange interaction and the degeneracies are removed. Our purpose is to derive an effective Hamiltonian in the limit where $|J| \gg |t_{ij}|$. We should exclude doubly occupied sites since they have higher energy of the order of J. The transfer term is written in a form which is similar to the 'correlated hopping' Hubbard model, where the transfer integrals are dependent on spin configurations at sites i and j. An important feature is that we have the terms such as $c^\dagger_{i\downarrow}c_{j\uparrow}$ and $c^\dagger_{i\uparrow}c_{j\downarrow}$. The following four processes should be considered, where we use the notation

$$\begin{pmatrix} d_i & d_j \\ s_i & s_j \end{pmatrix}, \tag{222}$$

for which d_i and s_i indicate spin state of the localized spin and the conduction electron at site i, respectively, and $-$ means no conduction electron:

$$\begin{pmatrix} \downarrow & \uparrow \\ - & \uparrow \end{pmatrix} \to \begin{pmatrix} \downarrow & \uparrow \\ \uparrow & - \end{pmatrix} \to \begin{pmatrix} \uparrow & \uparrow \\ \downarrow & - \end{pmatrix}, \tag{223}$$

$$\begin{pmatrix} \downarrow & \downarrow \\ - & \uparrow \end{pmatrix} \to \begin{pmatrix} \downarrow & \downarrow \\ \uparrow & - \end{pmatrix} \to \begin{pmatrix} \uparrow & \downarrow \\ \downarrow & - \end{pmatrix}, \tag{224}$$

$$\begin{pmatrix} \downarrow & \downarrow \\ - & \uparrow \end{pmatrix} \to \begin{pmatrix} \downarrow & \uparrow \\ - & \downarrow \end{pmatrix} \to \begin{pmatrix} \downarrow & \uparrow \\ \downarrow & - \end{pmatrix}, \tag{225}$$

$$\begin{pmatrix} \uparrow & \downarrow \\ - & \uparrow \end{pmatrix} \to \begin{pmatrix} \uparrow & \uparrow \\ - & \downarrow \end{pmatrix} \to \begin{pmatrix} \uparrow & \uparrow \\ \downarrow & - \end{pmatrix}. \tag{226}$$

These transfers are written in a unified way,

$$t_{ij}(1-n_{i\uparrow})c^\dagger_{i\downarrow}c_{j\uparrow}(1-n_{j\downarrow})(P_jP_i)_{\downarrow\uparrow}, \tag{227}$$

where a matrix $(P_i)_{\sigma\sigma'}$ is defined by

$$(P_i)_{\sigma\sigma} = \sigma S^z_i + \frac{1}{2} + \lambda \quad (\sigma = \uparrow, \downarrow), \tag{228}$$

$$(P_i)_{\uparrow\downarrow} = S^-_i, \quad (P_i)_{\downarrow\uparrow} = S^+_i, \tag{229}$$

or we can write

$$(P_i)_{\sigma\sigma'} = \mathbf{S}_i \cdot \sigma_{\sigma\sigma'} + (\frac{1}{2} + \lambda)\delta_{\sigma\sigma'}. \tag{230}$$

(λ is a constant.) $(P_iP_j)_{\downarrow\uparrow} = (P_i)_{\downarrow\uparrow}(P_j)_{\uparrow\uparrow} + (P_i)_{\downarrow\downarrow}(P_j)_{\downarrow\uparrow}$ in eq.(227) contributes to four terms above. Therefore the effective Hamiltonian for the conduction electrons is written in the form of a modified infinite-U model ($\lambda = 1$):[108]

$$H_{eff} = \sum_{ij\sigma\sigma'} t_{ij}(1-n_{i,-\sigma})c^\dagger_{i\sigma}c_{j\sigma'}(1-n_{j,-\sigma'})(P_iP_j)_{\sigma\sigma'}. \tag{231}$$

Now we investigate the ground state of this effective Hamiltonian. Let us consider the following statement.[111]

Theorem 4.2 We consider the Hamiltonian in eq.(231) on a one-dimensional (connected) lattice with open boundary condition. Suppose that $t = t_{ij}$ are non-zero for nearest-neighbor pairs (i, j) and $t < 0$. Then the ground state is unique for $N_e < N$ (where N_e and N are number of electrons and sites, respectively).

Proof It is easy to see that matrix elements of the Hamiltonian are non-positive if t is negative. This is because an electron cannot pass through another electrons since no doubly-occupied sites are allowed. It is also obvious that the matrix is irreducible because of the geometry (with periodic localized spins) of one-dimensional chain. To show this, we can employ the mathematical induction with respect to the number of sites.[111] Therefore the ground state is unique according to the Perron-Frobenius theorem. □

As a result of the Perron-Frobenius theorem, we have the ferromagnetic ground state with a positive eigenvector. This is a ferromagnetism due to the double exchange interaction. A similar discussion is possible for the antiferromagnetic Kondo coupling $J > 0$ which is going to be investigated in the next section.

4.3. *1D Kondo lattice in the limit of large J*

The Kondo lattice with the antiferromagnetic $J > 0$ is also mapped onto a Hubbard model with infinitely large on-site Coulomb interaction if we regard the local singlet as a hole.[109,110] Our model is defined on a one-dimensional lattice with open boundary condition. The ground state can be ferromagnetic due to the succesive exchange interactions (i.e. double exchange). We can easily emagine that the local singlets are moving along a chain and we should note that spin-flip process of the neighboring localized spins is never included in the infinite-J limit. This point is different from the case with the ferromagnetic $J < 0$ in the previous section. The matrix of the Hamiltonian is not necessarily irreducible in the zeroth order of t/J, which means that we have the spin degeneracy. For example, see the following process:

$$\begin{pmatrix} \uparrow & \downarrow & \downarrow \\ & & \uparrow \end{pmatrix} \to \begin{pmatrix} \uparrow & \downarrow & \downarrow \\ & \uparrow & \end{pmatrix} \to \begin{pmatrix} \uparrow & \uparrow & \downarrow \\ & \downarrow & \end{pmatrix} \to \begin{pmatrix} \uparrow & \uparrow & \downarrow \\ \downarrow & & \end{pmatrix}, \tag{232}$$

where the upper and lower parts indicate the localized spins and conduction electron, respectively. The localized spins are never exchanged.

Hence we should consider contributions of the order of t/J. There are two kinds of virtual processes: one is to make a local triplet and the other is to go through a doubly-occupied site. Both of them create next nearest neighbor hopping terms. (See below.)

$$\begin{pmatrix} \uparrow & \downarrow & \uparrow \\ & & \downarrow \end{pmatrix} \to \begin{pmatrix} \uparrow & \downarrow & \uparrow \\ & \downarrow & \end{pmatrix} \to \begin{pmatrix} \uparrow & \downarrow & \uparrow \\ \downarrow & & \end{pmatrix}, \tag{233}$$

$$\left(\begin{array}{ccc} \uparrow & \downarrow & \uparrow \\ & \uparrow & \downarrow \end{array}\right) \rightarrow \left(\begin{array}{ccc} \uparrow & \downarrow & \uparrow \\ & \downarrow\uparrow & \end{array}\right) \rightarrow \left(\begin{array}{ccc} \uparrow & \downarrow & \uparrow \\ \downarrow & \uparrow & \end{array}\right). \tag{234}$$

The former involves a spin flip and the latter causes no effect in the spin configuration. Therefore the effective Hamiltonian for $J > 0$ is written as, (See Ref.[109] for a mathematical derivation)

$$H = -t \sum_{\langle ij\rangle\sigma} \underline{\mathrm{f}}^{\dagger}_{i\sigma}\underline{\mathrm{f}}_{j\sigma} + t' \sum_{i\sigma} (\underline{\mathrm{f}}^{\dagger}_{i-1\sigma}\underline{\mathrm{n}}_{i}\underline{\mathrm{f}}_{i+1\sigma} + h.c.), \tag{235}$$

where $\underline{\mathrm{f}}_{i\sigma}$ are correlated operators: $\underline{\mathrm{f}}_{i\sigma} = f_{i\sigma}(1 - n_{i,-\sigma})$ and $\underline{\mathrm{n}}_i = \sum_\sigma \underline{\mathrm{f}}^{\dagger}_{i\sigma}\underline{\mathrm{f}}_{i\sigma}$. t' given by $t' = t^2/(2J)$ is the transfer parameter of three-site terms. The basis set for this effective Hamiltonian consists of states with various spin configurations without double occupancy. Thus it is easy to check that every off-diagonal element can be non-positive where they are $-t$ or $-t'$. Obviously the matrix of the Hamiltonian is irreducible since we have spin-flip processes. Hence a straightforward application of the Perron-Frobenius theorem leads to the following statement.

Theorem 4.3 Consider the Kondo lattice on a connected one-dimensional lattice with the open boundary condition. Suppose that $J > 0$ is antiferromagnetic. Then the spin degeneracy in the limit $J = \infty$ is lifted by the first-order perturbation in $1/J$. As a result the ground state is unique and ferromagnetic with the total spin $S = (N - N_e)/2$ for $N_e < N$ if J is large enough (where N is the number of sites and N_e is the number of conduction electrons).

The localized spin forms a singlet with a conduction electron at each site and the remaining spins are in a collective ferromagnetic state. The origin of the ferromagnetism is the double exchange as is the case for $J < 0$. Clearly this statement is not valid for the two- or three-dimensional models.

4.4. *Kondo lattice with one conduction electron*

Next application of the Perron-Frobenius theorem is the Kondo lattice with one conduction electron, which is also important to clarify the ground-state phase diagram.[112,113] It may be clear from the discussion above that the ground state has a ferromagnetic order in the limit of small carriers because of the double exchange. In fact, we can show the following proposition.[114]

Theorem 4.4 Let us consider the Kondo lattice Hamiltonian on a connected lattice given by

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + J \sum_i \mathbf{S}_i \cdot \sigma_i, \tag{236}$$

where σ_i denotes the spin operator of the conduction electron at site i. $t_{ij} = t > 0$ are assumed to vanish except between nearest-neighbor sites. Suppose that we have one conduction electron and we impose the open or periodic boundary

conditions. Then the ground state is unique for $J \neq 0$ (apart from the $2S+1$-fold spin degeneracy). The total spin of the ground state is given by

$$S = (N-1)/2 \text{ for } J > 0,$$
$$S = (N+1)/2 \text{ for } J < 0,$$

where N is the number of sites.

Proof First, we consider the case for $J > 0$ (antiferromagnetic coupling). If N is even, we work in the space $S^z = 1/2$, while if N is odd, our space has $S^z = 0$. The basis set consists of the states given as

$$\psi(j\sigma; \sigma_1, \cdots, \sigma_N) = \sigma c^\dagger_{j\sigma} |\sigma_1, \cdots, \sigma_N\rangle, \tag{237}$$

where $|\sigma_1, \cdots, \sigma_N\rangle$ indicates the localized spin configuration. Note that a spin-down conduction electron has a negative sign attached to wave functions. The Schrödinger equation reads

$$\begin{aligned} H\psi(j\sigma; \sigma_1, \cdots, \sigma_N) &= -\sum_i t_{ij} \psi(i\sigma; \sigma_1, \cdots, \sigma_N) + \frac{1}{4} J \sum_j \sigma_j \psi(j\sigma; \sigma_1, \cdots, \sigma_N) \\ &- \frac{1}{2} J \sum_{j(\sigma \neq \sigma_j)} \psi(j, -\sigma; \sigma_1, \cdots, \sigma_{j-1}, -\sigma_j, \sigma_{j+1}, \cdots, \sigma_N). \end{aligned} \tag{238}$$

It is straightforward to see that all the off-diagonal elements are non-positive for $J > 0$ and $t = t_{ij} > 0$. Since we have the spin-flip process between two localized spins within our basis set, the matrix of the Hamiltonian is shown to be irreducible. Then the lowest eigenvalue in the space $S^z = 0$ or $1/2$ (i.e. the ground state ψ), is unique with a positive eigenvector.

In order to show that the ground state has the total spin $S = (N-1)/2$, we construct a trial state ψ_{tri} with $S = (N-1)/2$ such that $\langle \psi_{tri} | \psi \rangle \neq 0$. From the construction of basis set, the following state

$$\psi_{ferr} = \psi(1, \uparrow; \downarrow, \uparrow, \cdots, \uparrow) + \psi(1, \downarrow; \uparrow, \uparrow, \cdots, \uparrow), \tag{239}$$

has $S = (N-1)/2$ in the space with $S^z = (N-1)/2$. Then we define

$$\psi_{tri} = (S^-)^n \psi_{ferr}, \tag{240}$$

where $n = [(N-1)/2]$ (=integer part of $(N-1)/2$). Since ψ_{tri} is a linear combination of basis states with non-negative weights, we have $\langle \psi_{tri} | \psi \rangle \neq 0$. Hence the ground state has $S = (N-1)/2$.

For the ferromagnetic coupling $J < 0$ (which is rather obvious compared to the case $J > 0$), we use the following basis states:

$$\psi(j\sigma; \sigma_1, \cdots, \sigma_N) = c^\dagger_{j\sigma} |\sigma_1, \cdots, \sigma_N\rangle, \tag{241}$$

with the same notation as before. The Schrödinger equation for these bases has the form

$$\begin{aligned} H\psi(j\sigma;\sigma_1,\cdots,\sigma_N) &= -\sum_i t_{ij}\psi(i\sigma;\sigma_1,\cdots,\sigma_N) + \frac{1}{4}J\sum_j \sigma\sigma_j\psi(j\sigma;\sigma_1,\cdots,\sigma_N) \\ &+ \frac{1}{2}J\sum_{j(\sigma\neq\sigma_j)}\psi(j,-\sigma;\sigma_1,\cdots,\sigma_{j-1},-\sigma_j,\sigma_{j+1},\cdots,\sigma_N). \end{aligned} \tag{242}$$

Obviously, the argument for $J > 0$ applies to the present case, and therefore we have a unique ground state with the total spin $S = (N+1)/2$. □

4.5. *Anderson lattice for* $N_e = N + 1$

Let us consider the Anderson lattice model at quarter filling with one extra electron, $N_e = |\Lambda| + 1$. Let $N = |\Lambda|$. We write again the Hamiltonian:

$$\begin{aligned} H &= -t\sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma} - \mu\sum_{i\sigma} n_{ci\sigma} \\ &+ V\sum_{i\sigma}(c^\dagger_{i\sigma}f_{i\sigma} + h.c.) + \epsilon_f\sum_{i\sigma} n_{fi\sigma} + U_f\sum_i n_{fi\uparrow}n_{fi\downarrow}. \end{aligned} \tag{243}$$

Here we do not include the Coulomb interactions between the conduction electrons because they are not important for our purpose. Since the Anderson (lattice) Hamiltonian is mapped onto the Kondo (lattice) Hamiltonian in the limit $\epsilon_f \to -\infty$ and $U_f \to \infty$, we can expect a ferromagnetic ground state for $N_e = N+1$.[115] Obviously the ground states are degenerate with respect to spin configurations in the limit $\epsilon_f \to -\infty$ (or $V \to 0$). Due to the perturbations in terms of V, the degeneracy will be partly lifted. We shall show that a first order perturbation in V lifts the degeneracy and a ferromagnetic state will be the ground state. Let us suppose that we can write the wave function in the form,

$$\psi = \psi_0 + \psi_1 + \psi_2 + \cdots. \tag{244}$$

ψ_0 is a zero-th order wave function which consists of basis states given as

$$\psi_{i\sigma;\{\sigma_n\}} = \sigma c^\dagger_{i\sigma}f^\dagger_{1\sigma_1}f^\dagger_{2\sigma_2}\cdots f^\dagger_{N\sigma_N}|0\rangle, \tag{245}$$

where $\{\sigma_n\}$ $(n = 1, 2, \cdots, N)$ denotes a set of spin configurations of f electrons. In the subspace $\{\psi_{i\sigma;\{\sigma_n\}}\}$, one conduction electron is moving around and we have a large spin degeneracy. The second term ψ_1 is of the order of V/ϵ_f and includes spin exchange processes between the conduction electrons and the f electrons. It is a priori not clear whether the degeneracy is lifted completely or we still have a degeneracy in the ground states. For simplicity, let us consider the lattice with open

boundary conditions. We make a statement in the following form.[b]

Theorem 4.5 Let us condider the Anderson lattice Hamiltonian with open boundary conditions. We assume that $N_e = N + 1$ and $U_f = \infty$. In the limit $\epsilon_f \to -\infty$, we have a degeneracy in the ground states with respect to spin configurations. The degeneracy is lifted due to the first order perturbation of the order of V/ϵ_f and then the ground state becomes unique. The ground state has the total spin $S = (N-1)/2$.

Proof We set $N_e = N + 1$. In the limit $\epsilon_f \to -\infty$, a wave function is written as a linear combination of the basis states $\{\psi_{i\sigma;\{\sigma_n\}}\}$:

$$\psi_{0,\sigma,\{\sigma_n\}} = \sum_i a^0_{i\sigma;\{\sigma_n\}} \psi_{i\sigma;\{\sigma_n\}}. \tag{246}$$

We have the large degeneracy with respect to $\{\sigma_n\}$ and σ. If we apply the Hamiltonian to $\psi_{i\sigma;\{\sigma_n\}}$, we obtain

$$\begin{aligned} H\psi_{i\sigma;\{\sigma_n\}} &= -t\sigma(c^\dagger_{i+1\sigma} + c^\dagger_{i-1\sigma}) f^\dagger_{1\sigma_1} \cdots f^\dagger_{N\sigma_N}|0\rangle \\ &+ V\sigma c^\dagger_{i\sigma} \sum_j (-1)^{j-1} c^\dagger_{j\sigma_j} f^\dagger_{1\sigma_1} \cdots f^\dagger_{j-1\sigma_{j-1}} f^\dagger_{j+1\sigma_{j+1}} \cdots f^\dagger_{N\sigma_N}|0\rangle \\ &+ N\epsilon_f \psi_{i\sigma;\{\sigma_n\}}. \end{aligned} \tag{247}$$

Hence ψ_1 consists of basis states given as

$$\psi_{i\sigma,j\sigma';\{\sigma_n\}} = (-1)^j \sigma c^\dagger_{i\sigma} c^\dagger_{j\sigma'} f^\dagger_{1\sigma_1} \cdots f^\dagger_{j-1\sigma_{j-1}} f^\dagger_{j+1\sigma_{j+1}} \cdots f^\dagger_{N\sigma_N}|0\rangle. \tag{248}$$

For $i = j$, the above definition means

$$\begin{aligned} \psi_{i\uparrow,i\downarrow;\{\sigma_n\}} &= \psi_{i\downarrow,i\uparrow;\{\sigma_n\}} \\ &= -(-1)^i c^\dagger_{i\downarrow} c^\dagger_{i\uparrow} f^\dagger_{1\sigma_1} \cdots f^\dagger_{i-1\sigma_{i-1}} f^\dagger_{i+1\sigma_{i+1}} \cdots f^\dagger_{N\sigma_N}|0\rangle. \end{aligned} \tag{249}$$

It is easy to see that ψ_1 is of order V/ϵ_f if we substitute $\psi = \psi_0 + \psi_1$ given as

$$\psi_0 = \sum_{i\sigma\{\sigma_n\}} a^0_{i\sigma;\{\sigma_n\}} \psi_{i\sigma;\{\sigma_n\}}, \tag{250}$$

$$\psi_1 = \sum_{i\sigma j\sigma'\{\sigma_n\}} a^1_{i\sigma j\sigma'\{\sigma_n\}} \psi_{i\sigma,j\sigma';\{\sigma_n\}}, \tag{251}$$

into the Schrödinger equation $H\psi = E\psi$. If we apply H to ψ_1, we have ψ_2 in which the conduction electrons excited from the f-level move to neighboring sites. However, ψ_2 is a state of the order of $(1/\epsilon_f)^2$, and we do not consider ψ_2 here.[c]

[b] We thank Prof. K. Ueda for his instructive comments.

[c] In Ref.[115], this property is not mentioned explcitly. Probably clever readers are already aware of the fact that $H\psi_1$ contains higher-order contributions. We should let the amplitude of a state such as

$$c^\dagger_{i\uparrow} c^\dagger_{k\uparrow} f^\dagger_{1\sigma_1} \cdots f^\dagger_{j-1\sigma_{j-1}} f^\dagger_{j+1\sigma_{j+1}} \cdots f^\dagger_{N\sigma_N}|0\rangle \quad (k \neq j) \tag{252}$$

to be 0. This means that the exchange of the conduction electrons with the same spin is not included.

With this definition in mind, it is clear that off-diagonal elements due to the kinetic part of the Hamiltonian are always non-positive ($-t < 0$ or 0) within the subspace spanned by $\{\psi_{i\sigma;\{\sigma_n\}}, \psi_{i\sigma,j\sigma';\{\sigma_n\}}\}$ for the open boundary conditions. It is also easy to obtain

$$\langle\psi_{i\sigma,j\sigma';\{\sigma_n\}}|H|\psi_{i\sigma;\{\sigma_n\}}\rangle = -V\delta_{\sigma'\sigma_j} \quad (i \neq j), \tag{253}$$

and

$$\langle\psi_{i\uparrow,i\downarrow;\{\sigma_n\}}|H|\psi_{i\sigma;\{\sigma_n\}}\rangle = -V\delta_{-\sigma\sigma_i}. \tag{254}$$

These two matrices are non-positive if $V > 0$. Thus we have shown that all the off-diagonal elements are non-positive in our subspace. Because of the geometry of the Anderson lattice, the Hamiltonian is irreducible. Hence, according to the Perron-Frobenius theorem, the ground state is unique and is a linear combination of basis states with positive coefficients.

In order to investigate the total spin, we have only to make a trial state with the total spin $S = (N-1)/2$ having a non-zero inner product with the ground state ψ. One example is

$$\psi_{tr} = (S^-)^n\psi_{ferr}, \tag{255}$$

where

$$\psi_{ferr} = \sum_i (-1)^{i-1}(c^\dagger_{i\uparrow}f^\dagger_{i\downarrow} - c^\dagger_{i\downarrow}f^\dagger_{i\uparrow})\prod_{j\neq i} f^\dagger_{i\uparrow}|0\rangle. \tag{256}$$

Therefore we can show that $S = (N-1)/2$. □

A mean field theory predicts the ferromagnetic phase near quarter filling[116] and suggests that the ferromagnetism survives in the thermodynamic limit.

4.6. *1D Kondo lattice with large Coulomb interaction* U

In this section, we investigate the effect of Coulomb interaction between the conduction electrons for the Kondo lattice Hamiltonian. The importance of the Coulomb interaction is now being appreciated for rare earth compounds. The Hamiltonian is written in the form

$$H = -t\sum_{\langle ij\rangle} c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} + J\sum_i \mathbf{S}_i\cdot\sigma_i, \tag{257}$$

where $\langle ij\rangle$ indicates a nearest-neighbor pair of sites and we denote $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$. We assume that the lattice is one-dimensional and we denote the number of sites as N and that of conduction electrons as N_e. We have considered the Kondo lattice Hamiltonian in the Chapter **2** for the half-filled band, where antiferromagnetic correlations are proved for $U > 0$. However, the exchange processes of the conduction electrons are reduced by the Coulomb interaction U away from the half filling, which may change the nature of spin correlations. Let us discuss the following proposition.[46]

Theorem 4.6 Assume that U is very large and $N_e < N$. Let us set the open

boundary condition. Then the ground state of the one-dimensional Kondo lattice in eq.(257) is unique and has the total spin

$$S = (N - N_e)/2 \text{ for } J > 0 \ ,$$
$$S = (N + N_e)/2 \text{ for } J < 0.$$

Proof We denote the operators of localized electrons as $f_{i\sigma}$ and $f^\dagger_{i\sigma}$. Suppose that U is infinitely large and that $J > 0$. We use the following representation for the basis states:

$$\begin{aligned} \psi(\{x_j\},\{\sigma_j\};\{s_i\}) &= \prod_{j=1}^{N_e} \sigma_j c^\dagger_{x_j\sigma_j} \prod_{j=1}^{N} f^\dagger_{js_j}|0\rangle \\ &\equiv \prod_{j=1}^{N_e} \sigma_j |x_1\sigma_1, x_2\sigma_2, \cdots, x_{N_e}\sigma_{N_e}\rangle \otimes |s_1, \cdots, s_N\rangle, \end{aligned} \tag{258}$$

where $\{x_i\}$ represent positions of the conduction electrons, $x_1 < x_2 < \cdots < x_{N_e}$, and $\{\sigma_i\}$ and $\{s_j\}$ denote spin configurations of the conduction and localized electrons, respectively. The wave function of this type is a generalization of that for the single-conduction electron case. Since U is infinite, an electron cannot pass through another electrons by the nearest-neighbor transfers. Then the Schrödinger equation for $\psi(\{x_j\},\{\sigma_j\};\{s_i\})$ reads

$$\begin{aligned} H\psi(\{x_j\},\{\sigma_j\};\{s_i\}) &= -t \sum_{\ell(x_\ell - 1 \neq x_{\ell-1})} \prod_i^{N_e} \sigma_i \\ &\times |x_1\sigma_1, \cdots, x_{\ell-1}\sigma_{\ell-1}, x_\ell - 1\sigma_\ell, x_{\ell+1}\sigma_{\ell+1}, \cdots, x_{N_e}\sigma_{N_e}\rangle \\ &\otimes |s_1 \cdots s_N\rangle \\ &- t \sum_{\ell(x_\ell + 1 \neq x_{\ell+1})} \prod_i^{N_e} \sigma_i \\ &\times |x_1\sigma_1, \cdots, x_{\ell-1}\sigma_{\ell-1}, x_\ell + 1\sigma_\ell, x_{\ell+1}\sigma_{\ell+1}, \cdots, x_{N_e}\sigma_{N_e}\rangle \\ &\otimes |s_1 \cdots s_N\rangle \\ &+ \frac{J}{2} \sum_{\ell, j(x_\ell = j, \sigma_\ell = -s_j)} \prod_i^{N_e} \sigma_i \\ &\times |x_1\sigma_1, \cdots, x_{\ell-1}\sigma_{\ell-1}, x_\ell - \sigma_\ell, x_{\ell+1}\sigma_{\ell+1}, \cdots, x_{N_e}\sigma_{N_e}\rangle \\ &\otimes |s_1 \cdots s_{j-1}, -s_j, s_{j+1}, \cdots, s_N\rangle \\ &+ (\textit{diagonal terms}) \\ &= (\textit{hopping terms}) \\ &- \frac{J}{2} \sum_{\ell, j(x_\ell = j, \sigma_\ell = -s_j)} \psi(\{x_i\}, \{\sigma_1, \cdots, \sigma_{\ell-1}, -\sigma_\ell, \sigma_{\ell+1}, \end{aligned}$$

$$\cdots \quad , \sigma_{N_e}\}; \{s_1 \cdots s_{j-1}, -s_j, s_{j+1}, \cdots, s_N\}) \\ + \quad (diagonal \;\; terms). \tag{259}$$

Obviously, the matrix elements due to the hopping terms and exchange interactions are non-positive (if $t > 0$ and $J > 0$). The matrix of the Hamiltonian is shown to be irreducible, for instance, in a similar manner to the double exchange model in the section **4.2**.[111] Therefore the Perron-Frobenius theorem implies that the ground state is unique.

To show that the ground state has the total spin $S = (N - N_e)/2$ for $J > 0$, we consider the following state

$$\psi_{tri} = \prod_{j=1}^{N_e} (c_{j\uparrow}^\dagger f_{j\downarrow}^\dagger - c_{j\downarrow}^\dagger f_{j\uparrow}^\dagger)(S^-)^n \prod_{i=N_e+1}^{N} f_{i\uparrow}^\dagger |0\rangle. \tag{260}$$

We can check that ψ_{tri} has a non-zero inner product with the ground state. Hence $S = (N - N_e)/2$.

For $J < 0$ (ferromagnetic case), the basis states are written in the form

$$\begin{aligned} \psi(\{x_j\}, \{\sigma_j\}; \{s_i\}) &= \prod_{j=1}^{N_e} c_{x_j \sigma_j}^\dagger \prod_{j=1}^{N} f_{j s_j}^\dagger |0\rangle \\ &\equiv \prod_{j=1}^{N_e} |x_1\sigma_1, x_2\sigma_2, \cdots, x_{N_e}\sigma_{N_e}\rangle \otimes |s_1, \cdots, s_N\rangle. \end{aligned} \tag{261}$$

Similarly, we can show that the ground state has $S = (N + N_e)/2$. □

We can say that this is the ferromagnetism due to the double exchange interaction. The above proposition indicates an example of the ferromagnetism induced by the Coulomb repulsion. In particular, a *metallic complete ferromagnetic state* is realized for $J < 0$. For a possible phase diagram of the 1D Kondo lattice with $U > 0$, see Ref.[46].

Now let us turn to the model where all the off-diagonal elements are non-positive and the Hamiltonian is, however, not (proved to be) irreducible. An example of such a model is given by the one-diemnsional Kondo Hamiltonian with two localized spins. We impose the open boundary condition for $N_e < N$. Suppose that the Coulomb repulsion U between the conduction electrons is very large, then the Hamiltonian has non-positive off-diagonal elements. Since we cannot show that the Hamiltonian is irreducible, we apply the Perron-Frobenius theorem for the general case to the two-impurity Kondo model. As a result, among the ground states there is one with a non-negative eigenvector. This eigenstate contains a ferromagnetic order, in which two localized spins show a parallel correlation.

4.7. *Nagaoka ferromagnetism*

A possible ferromagnetic state near half filling was pointed out by Nagaoka and Thouless.[117,118] This famous Nagaoka state can be recognized as an application of

the Perron-Frobenius theorem.[119] The Hamiltonian is given by the Hubbard model:

$$H = \sum_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{262}$$

where $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. We denote the number of sites and electrons as N and N_e, respectively. Nagaoka proved the following statement.

Theorem 4.7(Nagaoka) Assume that t_{ij} is nonvanishing only between nearest-neighbor sites, which is denoted by t. The crystal structure is simple cubic, body-centered cubic, face centered cubic, or hexagonal closed packed. Then the ferromagnetic state with the maximum total spin is the ground state of the system for $N_e = N - 1$, $U = \infty$, and $t > 0$.

Remark The ferromagnetic state is given by filling up the band for up electrons except one level at the band top. This state has

$$S = S_{max} = \frac{1}{2} N_e, \quad S^z = \pm S, \tag{263}$$

$$E = -zt, \tag{264}$$

where z is the number of nearest-neighbor sites. The lattice structures mentioned above have the property that the Hamiltonian corresponding to a given lattice is irreducible. Let us consider the three-site ring with two electrons: $d_1(\uparrow)d_2(\downarrow)d_3(-)$. If a hole goes around a loop, we obtain $d_1(\downarrow)d_2(\uparrow)d_3(-)$. Thus two electrons with antiparallel spins are exchanged. It is also easy to see that we can rearrange spins in the four-site ring from one configuratin to another for any numbers of up- and down-spin electrons. (Note that this is not possible for the five-site ring.) Then by the induction the irreducibility of the Hamiltonian is proved, i.e. any two states in the basis set is connected by the succesive application of the Hamiltonian.[117]
Proof We use the representation of basis states given by Nagaoka:

$$\psi_{i\alpha_i} = (-1)^i c^\dagger_{1\sigma_1} c^\dagger_{2\sigma_2} \cdots c^\dagger_{i-1\sigma_{i-1}} c^\dagger_{i+1\sigma_{i+1}} \cdots c^\dagger_{N\sigma_N} |0\rangle, \tag{265}$$

where α_i denotes the set $(\sigma_1, \sigma_2, \cdots, \sigma_{i-1}, \sigma_{i+1}, \cdots, \sigma_N)$ and $|0\rangle$ is the vacuum state. We can work in the space with fixed S^z. Then the Schrödinger equation is written in the form:

$$\begin{aligned} H\psi_{i\alpha_i} &= \sum_j t_{ij} (-1)^{2i-j-1} c^\dagger_{1\sigma_1} \cdots c^\dagger_{j-1\sigma_{j-1}} c^\dagger_{j+1\sigma_{j+1}} \cdots c^\dagger_{N\sigma_N} |0\rangle \\ &= -\sum_j t_{ij} \psi_{j\alpha_j}. \end{aligned} \tag{266}$$

Hence the off-diagonal elements are non-positive. As we have noted before that the Hamiltonian is irreducible, the straightforward application of the Perron-Frobenius theorem states that the ground state is unique and given by a linear combination

of all the states $\psi_{i\alpha_i}$ with positive amplitudes in the space $S^z = 0$ or $1/2$. From the definition of basis states, the ground state has $S = (N-1)/2$. □

Remark Since the square cubic (sc) and the body-centered cubic (bcc) with nearest-neighbor hoppings are bipartite, we can change t into $-t$ by attaching (-1) to wavefunctions on the B sublattice. Hence

Corollary The ground state for sc and bcc has the maximum total spin for $N_e = N-1$, $U = \infty$, and $t = t_{ij} < 0$.

An extension of the Nagaoka's theorem is possible where the restriction on the lattice can be relaxed.[119] Let us give a definition and theorems.

Definition A finite lattice Λ is said to be irreducible with respect to $\{t_{ij}\}$ if the Hamiltonian corresponding to Λ is irreducible in each sector with fixed S^z.[d]

Theorem 4.8 Let us consider the Hubbard model in eq.(262) with $\{t_{ij} \geq 0\}$, $U = \infty$, and $N_e = N-1$. Then there exist at least N states with $S = (N-1)/2$.

Theorem 4.9 Consider the Hubbard model in eq.(262) with $\{t_{ij} \geq 0\}$, $U = \infty$, and $N_e = N-1$. Let us further assume that the lattice Λ is irreducible. Then the ground state is unique apart from the trivial N-fold degeneracy and has $S = (N-1)/2$.

Theorem 4.8 is proved by the Perron-Frobenius theorem for the general case. A set of the lattices mentioned in *Theorem 4.9* include the lattice sturctures in *Theorem 4.7*, the triangular lattice and the lattices which consist of three-site loops and four-site loops. It is not clear whether the crystal of C_{60} is irreducible or not since C_{60} has five-site loops and six-site loops. It is impossible to generalize the statement for more than one hole. The ferromagnetism near half filling in the thermodynamic limit has been investigated by many authors[120,121,122,123,124,125,126] being a hot topic in strongly-correlated electrons. For the one-dimensional chain, the ferromagnetic state is among the ground states and is not necessarily unique.

4.8. *A zigzag Anderson lattice:* $N_e \leq N$

For the one-dimensional Hubbard model, the ground states are degenerate with respect to spin configurations for $U = \infty$. This degeneracy is easily lifted toward the ferromagnetic state by the hybridization with the higher-energy levels, which is examined in this section.[127] Our Hamiltonian is the Anderson lattice model given as

$$H = \sum_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U_c \sum_i n_{ci\uparrow} n_{ci\downarrow} + \Delta \sum_{i\sigma} f^\dagger_{i\sigma} f_{i\sigma}$$

[d] We use the terminology *irreducible* inplace of *connected* since we have used *connected* in the Chapter **2**.

$$+ \quad V\sum_{i\sigma}[f^\dagger_{i\sigma}(c_{i\sigma}+c_{i+1\sigma})+h.c.]+U_f\sum_i n_{fi\uparrow}n_{fi\downarrow}, \tag{267}$$

where U_c and U_f denote the strength of Coulomb interactions among the conduction electrons and f electrons, respectively, and the level of f electrons is denoted by Δ. Other notations are standard for the Anderson model. We call this model the zigzag Anderson lattice here. The hopping parameters t_{ij} are non-zero between nearest-neighbor sites and assumed to be positive $t = t_{ij} > 0$. An extension to the two or three dimensional cases is straightforward. For the two-dimensional space, the Hamiltonian is written as

$$\begin{aligned} H &= \sum_{ij} t_{ij}c^\dagger_{i\sigma}c_{j\sigma} + U_c\sum_i n_{ci\uparrow}n_{ci\downarrow} + \Delta\sum_{i\mu(=x,y)\sigma} f^\dagger_{i+\frac{1}{2}\mu\sigma}f_{i+\frac{1}{2}\mu\sigma} \\ &+ V\sum_{i\mu\sigma}[f^\dagger_{i+\frac{1}{2}\mu\sigma}(c_{i\sigma}+c_{i+\mu\sigma})+h.c.]+U_f\sum_{i\mu} n_{fi+\frac{1}{2}\mu\uparrow}n_{f1+\frac{1}{2}\mu\downarrow}, \end{aligned} \tag{268}$$

where μ denotes a unit vector in the x and y directions. Let us consider the case in which $\Delta \gg t$ and $0 < V/\Delta \ll 1$. We suppose that U_c and U_f are large. Then in the limit $V/\Delta \to 0$, the ground states are highly degenerate. Our purpose is to show that the degeneracy is lifted toward the ferromagnetic state by a perturbation in V/Δ. We use the following representation for the basis states up to the order of V/Δ:

$$\psi^0(\sigma_1\cdots\sigma_N) = c^\dagger_{1\sigma_1}c^\dagger_{2\sigma_2}\cdots c^\dagger_{N\sigma_N}|0\rangle, \tag{269}$$

$$\psi^1(i\sigma;\sigma_1\cdots\sigma_{i-1}\sigma_{i+1}\cdots\sigma_N) = (-1)c^\dagger_{1\sigma_1}\cdots c^\dagger_{i-1\sigma_{i-1}}f^\dagger_{i\sigma}c^\dagger_{i+1\sigma_{i+1}}\cdots c^\dagger_{N\sigma_N}|0\rangle, \tag{270}$$

$$\psi^1(i\sigma;\sigma_1\cdots\sigma_i\sigma_{i+2}\cdots\sigma_N) = (-1)c^\dagger_{1\sigma_1}\cdots c^\dagger_{i\sigma_i}f^\dagger_{i\sigma}c^\dagger_{i+2\sigma_{i+2}}\cdots c^\dagger_{N\sigma_N}|0\rangle. \tag{271}$$

The ground state wavefunction is a linear combination of these bases. The matrix elements are given by

$$\langle\psi^1(i\sigma;\sigma_1\cdots\sigma_{i-1}\sigma_{i+1}\cdots\sigma_N)|H|\psi^0(\sigma_1\cdots\sigma_N)\rangle = -V\delta_{\sigma\sigma_i}, \tag{272}$$

$$\langle\psi^1(i-1\sigma;\sigma_1\cdots\sigma_{i-1}\sigma_{i+1}\cdots\sigma_N)|H|\psi^0(\sigma_1\cdots\sigma_N)\rangle = -V\delta_{\sigma_i\sigma_{i+1}}, \tag{273}$$

$$\langle\psi^1(i\sigma;\sigma_1\cdots\sigma_i\sigma_{i+2}\cdots\sigma_N)|H|\psi^1(i\sigma;\sigma_1\cdots\sigma_{i-1}\sigma_{i+1}\cdots\sigma_N)\rangle = -t\delta_{\sigma_i\sigma_{i+1}}. \tag{274}$$

Then the matrix is non-positive (for $V > 0$ and $t > 0$) in our basis set and is shown to be irreducible because we have spin-flip processes between nearest-neighbor sites. In summary we can say:

Theorem 4.10 Consider the zigzag Anderson lattice in eq.(267) at quarter filling $N_e = N$. Let us assume that U_c and U_f are infinitely large and the hopping parameters t_{ij} are non-zero and positive only between nearest-neighbor sites. Assume further that $V > 0$, $\Delta > 0$, $V/\Delta \ll 1$ and $t/\Delta \ll 1$ (for $t = t_{ij} > 0$). Then the ground state has the maximum total spin $S = N_e/2$.

If we restrict ourselves to the one-dimensional space, we can expect the ferromagnetism for less than quarter filling.[127] Let us examine this case. The basis set is

composed of states which are up to the order of V/Δ. In the limit $V/\Delta = 0$, our representation is an extension of that given by Nagaoka:

$$\psi^0(i_1\sigma_1, \cdots, i_n\sigma_n) = (-1)^{i_1+\cdots+i_n} c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} \cdots c^\dagger_{i_n\sigma_n} |0\rangle, \tag{275}$$

where $n = N_e$. In the subspace spanned by the states $\psi^0(i_1\sigma_1, \cdots, i_n\sigma_n)$, we have

$$\begin{aligned} H\psi^0(i_1\sigma_1, \cdots, i_n\sigma_n) \quad = \quad & -t \sum_{j(i_{j-1}\neq i_j-1)} \psi^0(i_1\sigma_1, \cdots, i_{j-1}\sigma_{j-1}, i_j - 1\sigma_j, \\ & i_{j+1}\sigma_{j+1}, \quad \cdots, i_n\sigma_n) \\ & -t \sum_{j(i_{j+1}\neq i_j+1)} \psi^0(i_1\sigma_1, \cdots, i_{j-1}\sigma_{j-1}, i_j + 1\sigma_j, \\ & i_{j+1}\sigma_{j+1}, \quad \cdots, i_n\sigma_n). \end{aligned} \tag{276}$$

Here the non-zero matrix elements are negative $-t < 0$. In the order of V/Δ we should consider the following two processes:

$$\begin{aligned} s_i(\sigma)d_i(-)s_{i+1}(\sigma') &\to s_i(\sigma)d_i(\sigma')s_{i+1}(-) \to s_i(-)d_i(\sigma')s_{i+1}(\sigma) \\ &\to s_i(\sigma')d_i(-)s_{i+1}(\sigma), \\ s_i(-)d_i(-)s_{i+1}(\sigma) &\to s_i(-)d_i(\sigma)s_{i+1}(-) \to s_i(\sigma)d_i(-)s_{i+1}(-) \\ &\to s_i(-)d_i(-)s_{i+1}(\sigma). \end{aligned}$$

The former can be taken into account with the non-positive matrix elements by using the Nagaoka representation for the basis states as in eqs.(270) and (271). The latter process gives rise to positive matrix elements which may cause a mismatch in the proof. However, this process contributes to give an effective transfer term without producing any effects on the spin configurations, which means that the spin-flip processes are not accompanied. If $t \gg V^2/\Delta$ (or $t \gg V$), we can neglect it since $V/\Delta \cdot V/t$ is much smaller than 1.[e] Therefore we can say in the following way (although it is not perfectly mathematical which means that the Hamiltonian is nearly non-positive):

Theorem 4.11 We consider the one-dimensional zigzag Anderson lattice Hamiltonian for $N_e \leq N$ with same conditions stated in *Theorem 4.10*. Suppose further that $t \gg V^2/\Delta$ and impose the open boundary condition. Then the ground state has the maximum total spin $S = N_e/2$.

We can modify the structure of hybridizations so that the ground state remains ferromagnetic at quarter filling $N_e = N$. For instance one can consider the Anderson

[e] This kind of argument can be applied to the Anderson lattice for $N_e = N + 1$ in the section **4.5**. The basis states of type in eq.(252) produce the exchange of electrons with the same spin and then we have positive matrix elements which cannot be removed. However, these contributions make no effects on the spin configurations of other electrons, leading to an effective hybridization. Hence we can again neglect the basis states in eq.(252) if $|V/\epsilon_f| \ll 1$ and $|t/\epsilon_f| \ll 1$.

lattice with 'mountain structure' given as

$$\begin{aligned} H &= \sum_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U_c \sum_i n_{ci\uparrow} n_{ci\downarrow} + \Delta \sum_{i\sigma} f^\dagger_{i\sigma} f_{i\sigma} \\ &+ V \sum_{i\sigma} [f^\dagger_{i\sigma} (c_{i-1\sigma} + c_{i\sigma} + c_{i+1\sigma}) + h.c.] + U_f \sum_i n_{fi\uparrow} n_{fi\downarrow}. \end{aligned} \tag{277}$$

Other extensions may be possible.

4.9. *1D Hubbard model*

Because of the restricted geometry of the one-dimensional models, it is shown that the ground state of some 1D models is a singlet for an even number of electrons for the appropriate boundary conditions. Lieb and Mattis have shown that the ground state is a singlet for the interactions of diagonal type.[128] In this section we shall consider the one-dimensional Hubbard model and the t-J model from the viewpoint of the Perron-Frobenius theorem.[129] The Hamiltonian is given by

$$H = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{278}$$

where $\langle ij \rangle$ indicates nearest-neighbor sites on a one-dimensional chain and we assume that $t > 0$ and $J \geq 0$. Let us investigate the following proposition.

Theorem 4.12 The ground state of the Hamiltonian (278) is unique and a singlet for an even number of electrons in the following cases for $t > 0$ and $J \geq 0$.
(1) $N_e = 4m + 2$ (m=integer) for the periodic boundary condition or the open boundary condition.
(2) $N_e = 4m$ for the antiperiodic boundary condition or the open boundary condition.
(We exclude the case in which $U = \infty$ and $J = 0$.)

Proof We can work in each sector with fixed S^z. For simplicity let us work in the subspace with $S^z = 0$. It is convenient to use the representation for the basis states by Lieb:[48]

$$\begin{aligned} \psi_{\alpha\beta} &= \psi^\uparrow_\alpha \otimes \psi^\downarrow_\beta \\ &= c^\dagger_{i_1\uparrow} \cdots c^\dagger_{i_n\uparrow} c^\dagger_{j_1\downarrow} \cdots c^\dagger_{j_n\downarrow} |0\rangle, \end{aligned} \tag{279}$$

where $n = N_e/2$, and $\alpha = (i_1 \cdots i_n)$ and $\beta = (j_1 \cdots j_n)$ indicate the locations of electrons in the real space for $i_1 < i_2 < \cdots < i_n$ and $j_1 < j_2 < \cdots < j_n$. Obviously, all the off-diagonal matrix elements due to electron hoppings are non-positive $-t < 0$. It is also easy to see that the off-diagonal elements due to the nearest-neighbor exchange interaction are non-positive. For instance, when we can exchange the up-spin electron at site i_m and the down-spin electron at site j_ℓ, we

obtain

$$\begin{aligned} S^-_{i_m} S^+_{j_\ell} \quad & c^\dagger_{i_1\uparrow}\cdots c^\dagger_{i_n\uparrow} c^\dagger_{j_1\downarrow}\cdots c^\dagger_{j_n\downarrow}|0\rangle \\ = \quad & c^\dagger_{i_1\uparrow}\cdots c^\dagger_{i_{m-1}\uparrow} c^\dagger_{i_m\downarrow} c^\dagger_{i_{m+1}\uparrow}\cdots c^\dagger_{i_n\uparrow} c^\dagger_{j_1\downarrow}\cdots c^\dagger_{j_{\ell-1}\downarrow} c^\dagger_{j_\ell\uparrow} c^\dagger_{j_{\ell+1}\downarrow}\cdots c^\dagger_{j_n\downarrow}|0\rangle \\ = \quad & -c^\dagger_{i_1\uparrow}\cdots c^\dagger_{i_{m-1}\uparrow} c^\dagger_{i_\ell\uparrow} c^\dagger_{i_{m+1}\uparrow}\cdots c^\dagger_{i_n\uparrow} c^\dagger_{j_1\downarrow}\cdots c^\dagger_{j_{\ell-1}\downarrow} c^\dagger_{j_m\downarrow} c^\dagger_{j_{\ell+1}\downarrow}\cdots c^\dagger_{j_n\downarrow}|0\rangle. \end{aligned} \tag{280}$$

The boundary conditions depend upon the number of electrons so that the matrix elements are non-positive. It is clear that the Hamiltonian is irreducible except the case in which $U = \infty$ and $J = 0$. Therefore the Perron-Frobenius theorem indicates that the ground state is unique and is continuous with respect to U and $J \geq 0$. The ground state is a singlet since it is connected to the non-interacting case where $U = 0$ and $J = 0$. □

As is shown in *Theorem 4.12* the ground state has definite signs in a linear combination of basis states, which makes the one-dimensional systems tractable by analytical and numerical methods.

Lastly, we consider an unrealistic model which means the 1D t-J model with the ferromagnetic interaction $J < 0$:

$$H = -t \sum_{\langle ij\rangle\sigma} (1 - n_{i,-\sigma}) c^\dagger_{i\sigma} c_{j\sigma} (1 - n_{j,-\sigma}) + J \sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \tag{281}$$

If we use the basis states given by

$$\psi(i_1\sigma_1, \cdots, i_n\sigma_n) = c^\dagger_{i_1\sigma_1} c^\dagger_{i_2\sigma_2} \cdots c^\dagger_{i_n\sigma_n}|0\rangle, \tag{282}$$

where $n = N_e$, all the off-diagonal elements are non-positive for $t > 0$ and $J < 0$ if we impose appropriate boundary conditions. Hence we can show in a similar way that the ground state has the maximum total spin. If we make the electron-hole transformation for the down-spin electrons in the ferromagnetic t-J model in eq.(281), we can obtain the Hamiltonian which exhibits exactly a superconducing ground state. Let us consider a 'correlated hopping' Hubbard model with the attractive interaction given as[88]

$$\begin{aligned} \tilde{H} \quad = \quad & -t \sum_{\langle ij\rangle} [n_{i\downarrow} c^\dagger_{i\uparrow} c_{j\downarrow} n_{j\downarrow} + (1 - n_{i\uparrow}) c^\dagger_{i\downarrow} c_{j\downarrow} (1 - n_{j\uparrow})] \\ - \quad & t_p \sum_{\langle ij\rangle} (c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow} + c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} c_{i\downarrow} c_{i\uparrow}) \\ + \quad & V \sum_{\langle ij\rangle} n_i n_j - \epsilon_0 \sum_{i\sigma} n_{i\sigma} + const, \end{aligned} \tag{283}$$

where $t_p = -J/2$, $V = J/4$ and $\epsilon_0 = J/2$. The up-spin electrons should be accompanied with the down-spin electrons in this Hamiltonian. Since $\mathbf{S}^2$ and S^z commute with H, the η-spin operators $\mathbf{J}^2$ and J^z commute with $\tilde{H}$. Let N_e and N be the

number of electrons and that of sites, respectively. Suppose that we work in the space with $S^z = 0$ (S^z commutes with $\tilde{H}$). According to the partial electron-hole transformation, J is transformed to S and we have

$$J = N_e/2 = N/2, \quad J^z = (N_e - N)/2. \tag{284}$$

Hence there is ODLRO because of *Theorem 2.13*. Note that the ground state has the same quantum numbers of J and J^z as the Yang's η-paring state. In fact, the ground state of $\tilde{H}$ is given by

$$\psi_\eta = A(J^+)^{N_e/2}|0\rangle, \tag{285}$$

because the ferromagnetic ground state for H in eq.(281)

$$\psi_{ferr} = A(S^+)^{N_e/2}|\downarrow\downarrow\cdots\downarrow\rangle \tag{286}$$

is transformed to the η-paring state ψ_η. A class of the attractive Hubbard models for which the ground state is given by the Yang's state has been investigated in Refs.[130,131].

5. Concluding remarks

We have discussed the applications of the reflection positivity in the spin space and the Perron-Frobenius theorem. The reflection positivity in the spin space is intrinsic for the Heisenberg model, the Hubbard model and the Kondo lattice at half filling. The reflection positivity in the spin space means that the matrix representation of the ground state eigenfunction is positive definite. One may wonder why this property is called the reflection positivity. In order to answer this question, let us examine the reflection positivity in field theory.[50,132,133,134] We denote a set of basis states with spin-σ electrons as X^σ which are finite-dimensional vector spaces. We denote a set of linear transformations on X^σ as A_σ, which are represented as matrices. We write $A = A_\uparrow + A_\downarrow$. A can be regarded as C^*-algebra[135] with the standard operator norm[f]

$$||M|| = sup\{||Mu||; u \in X^\sigma, ||u|| = 1\} \quad (M \in A_\sigma). \tag{287}$$

[f] A C^*-algebra is an algebra which has the algebraic structure of bounded operators acting on a Hilbert space. A vector space A with coefficient field $\mathbf{C}$ (the field of complex numbers) is called *-algebra if A is a ring and a mapping (called an involution) $X \in A \to X^* \in A$ is defined with the properties:

(1) $X^* = X$,
(2) $(XY)^* = Y^*X^*$,
(3) $(\alpha X + \beta Y)^* = \alpha^* X^* + \beta^* Y^*$.

The algebra A is called normed algebra if we can associate a real number $||X||$ to each element $X \in A$, satisfying the criterions of norm. A normed algebra A with involution is a Banach *-algebra if A is complete and has the property $||X|| = ||X^*||$. A Banach*-algebra is called a C^*-algebra if $||X^*X|| = ||X||^2$ holds for all $X \in A$.

Suppose that there is a one to one and continuous map $\theta : A_\uparrow \to A_\downarrow$ such that

$$\theta(M+N) = \theta(M) + \theta(N), \tag{288}$$

$$\theta(\alpha M) = \alpha^* \theta(M), \tag{289}$$

for $M, N \in A_\uparrow$ and $\alpha \in \mathbf{C}$. α^* denotes its complex conjugate. Let us denote a linear functional on A as $\langle\cdot\rangle$. Then we can define the reflection positivity in the following way:[132,133,134]

Definition Let A be a C^*-algebra with an identity and $A_\pm$ be subalgebras of A. Suppose that there is a one to one and continuous map $\theta : A_+ \to A_-$ such that

$$\langle \theta(M) M \rangle \geq 0 \quad (\forall M \in A_+). \tag{290}$$

Then $\langle\cdot\rangle$ is said to be reflection positive with respect to θ.

We define the functional $\langle\cdot\rangle$ as

$$\langle F \rangle = TrF \quad (F \in A). \tag{291}$$

When the number of spin-up electrons is equal to that of spin-down electrons, $A_\uparrow$ and $A_\downarrow$ are identical as sets. If we define θ as $\theta(M) = I_{\downarrow\uparrow} M^\dagger I_{\uparrow\downarrow}$ $(M \in A_\uparrow)$, we obtain

$$\langle \theta(M) M \rangle = TrM^\dagger M \geq 0, \tag{292}$$

$I_{\sigma,-\sigma}$ are identity mapping $A_{-\sigma} \to A_\sigma$ for $\sigma =\uparrow$ or $\downarrow$. Thus $\langle\cdot\rangle$ is reflection positive with respect to $\theta(M) = M^\dagger$. This is a trivial example. Let us investigate the reflection positivity with respect to the ground state. As is shown in the section **2.1**, the eigenfunction can be regarded as a mapping

$$C : X^\downarrow \to X^\uparrow, \tag{293}$$

if we write the eigenfunction in the form $\psi = \sum_{\alpha\beta} C_{\alpha\beta}\psi_{\alpha\beta}$. Then we can define the following θ:

$$\theta(M) = C^\dagger M^\dagger C \quad (M \in A_\uparrow). \tag{294}$$

If C is hermitian and positive definite, θ is one to one (injective).[g] For positive definite C, $\langle\theta(M)M\rangle = TrC^\dagger M^\dagger CM \geq 0$, i.e. $\langle\cdot\rangle$ is reflection positive with respect to θ in eq.(294).[hi] Hence we can say that the ground state has reflection positivity if the coefficient matrix C of the ground state is positive definite.

The second part of this paper has been devoted to discuss the applications of the Perron-Frobenius theorem which has a long history since the work by Lieb and Mattis. Theory of irreducible non-negative matrices was developed to be a beautiful

[g] Since C has inverse C^{-1}, $\theta(M) = 0$ implies $M = 0$, i.e. Ker$\theta = \{0\}$.

[h] Strictly speaking, we should identify $M \in A_\uparrow$ with $M \in A_\downarrow$ if we compare $\langle\theta(M)M\rangle$ with the energy eq.(18).

[i] θ in eq.(294) is not morphism, i.e. $\theta(MN) = \theta(M)\theta(N)$ does not hold.

theory. The Perron-Frobenius theorem indicates that the ground state eigenfunction has no nodes and thus in most cases this theorem predicts ferromagnetic ground states.

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