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Entanglement in Valence-Bond-Solid States and Quantum Search

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Ying Xu

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Ying Xu

We, the dissertation committee for the above candidate for the Doctor of Philosophy degree, hereby recommend acceptance of this dissertation.

Vladimir E. Korepin – Dissertation Advisor
Professor, C.N. Yang Institute for Theoretical Physics

Warren D. Siegel – Chairperson of Defense
Professor, C.N. Yang Institute for Theoretical Physics

Dominik A. Schneble
Assistant Professor, Department of Physics and Astronomy

Barry McCoy
Distinguished Professor, C.N. Yang Institute for Theoretical Physics

Peter van Nieuwenhuizen
Distinguished Professor, C.N. Yang Institute for Theoretical Physics

Alexander Kirillov, Jr.
Associate professor
Department of Mathematics

This dissertation is accepted by the Graduate School.

Lawrence Martin
Dean of the Graduate School

Abstract of the Dissertation

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The present dissertation covers two independent subjects: i) The quantum entanglement in Valence-Bond-Solid states, and ii) quantum database search algorithms. Both subjects are presented in a self-contained and pedagogical way.

i) The first chapter is a through introduction to the subject of quantum entanglement in Valence-Bond-Solid (VBS) states defined on a lattice or graph. The VBS state was first introduced as the ground state of the celebrated Affleck-Kennedy-Lieb-Tasaki (AKLT) spin chain model in statistical mechanics. Then it became essential in condensed matter physics, quantum information and measurement-based quantum computation. Recent studies elucidated important entanglement properties of the VBS state. We start with the definition of a general AKLT model and the construction of VBS ground states. A subsystem is introduced and described by the density matrix. Exact spectrum properties of the density matrix are proved and discussed. Density matrices of 1-dimensional models are diagonalized and the entanglement entropies (the von Neumann entropy

and Rényi entropy) are calculated. The entropies take saturated value and the density matrix is proportional to a projector in the large subsystem limit.

ii) The second chapter is a detailed introduction to the subject of quantum database search algorithms. The problem of searching a large database (a Hilbert space) for a target item is performed by the famous Grover algorithm which locates the target item with probability 1 and a quadratic speed up compared with the corresponding classical algorithm. If the database is partitioned into blocks and one is searching for the block containing the target item instead of the target item itself, then the problem is referred to as partial search. Partial search trades accuracy for speed and the most efficient version is the Grover-Radhakrishnan-Korepin (GRK) algorithm. The target block can be further partitioned into sub-blocks so that GRK can be performed in a sequence called a hierarchy. We formulate the Grover search and GRK partial search and prove that a GRK hierarchy is less efficient than a direct GRK partial search.

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Chapter 1

Entanglement in Valence-Bond-Solid States

1.1 Introduction

The fields of statistical mechanics, condensed matter physics and quantum information theory share a common interest in the study of interacting quantum many body systems. The concept of **entanglement** in quantum mechanics has significant importance in all these areas. Roughly speaking, entanglement [41] is a phenomenon of quantum mechanical nature in which quantum states of physical systems are linked together so that one system can not be adequately described without full mention of its counterpart, even when the individual systems may be spatially separated. Entanglement becomes particularly interesting in a many body interacting system where a subsystem (also a physical system by itself) may strongly correlate with its environment (other parts of the system) in terms of observable physical properties. The correlations may reject the principle of local realism, which states that information about the state of a system can only be mediated by interactions in its immediate surroundings (neighbors). The characteristic length of entanglement may be diverging while the usual correlation length remains finite [49]. Quantum entanglement is a fundamental measure of how much quantum effects we can observe and use to control one quantum system by another, and it is the primary resource in emerging technologies of quantum computation and quantum information processing [6]. Entanglement properties play an important role in condensed matter physics, such as phase transitions and macroscopic properties of solids [43, 44]. At the same time, it also prompts some of the more philosophically oriented discussions concerning quantum theory.

Much of current research seeks to elucidate quantum entanglement in a

variety of interacting systems. Extensive research has been undertaken to investigate quantum entanglement in strongly correlated states such as spin chains, correlated electrons, interacting bosons as well as other models. (See [3, 16, 17, 20, 26, 30, 31, 34, 38, 39, 42, 45, 46, 49] for reviews and references.) A general approach studies the density matrix of a certain subsystem of a strongly entangled state. The spectrum of the density matrix and the derived entropy functions serve as measures of entanglement. The von Neumann entropy and Rényi entropy are typical quantifications of entanglement. These characteristic functions may depend on the physical parameters (size, coupling constants, external fields, *etc.*) in various different ways. An area law for the von Neumann entropy in harmonic lattice systems has been extensively studied [8, 9, 28], which states that the entropy scales proportional to the size (area) of the boundary of the subsystem. (For comparison, a classical Boltzmann entropy is an extensive quantity proportional to the size (volume) of the physical system.) The entropy of the whole system vanishes if the system is in a pure state (usually the unique ground state), but it can be positive for a subsystem. (The density matrix of the whole system is pure but the density matrix of a subsystem usually takes the form of mixed states.) Much insight in understanding entanglement of quantum systems has been obtained by studying exactly solvable models in statistical mechanics, in which it is possible to solve the subsystem density matrix and calculate the entropy exactly. This chapter is devoted to one particular model – the AKLT model.

In 1987, I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki proposed a spin interacting model known as the AKLT model [1, 2]. The model consists of spins on a lattice and the Hamiltonian describes interactions between nearest neighbors. The Hamiltonian density is a linear combination of projectors. Each projector is written as a polynomial of the inner product of a pair of interacting spin vectors. The model is similar to the Heisenberg anti-ferromagnet with a gap. The authors (AKLT) of [1, 2] found the exact ground state, which has an exponentially-decaying correlation function and a finite energy gap. In their early works, authors discussed the 1-dimensional AKLT lattices with open and periodic boundary conditions and 2-dimensional models such as the Hexagonal lattice. This model has been attracting enormous research interests since then [10, 13, 18, 32, 33, 36]. It can be defined and solved in higher dimensional and arbitrary lattices [2, 12, 35, 47] and generalizable to the inhomogeneous (non-translational invariant) case (spins at different lattice sites may take different values) and an arbitrary graph [36, 52]. Given certain conditions (as to be described later), the ground state has proven to be unique [4, 36]. It is known as the Valence-Bond-Solid (VBS) state. The VBS state lies at the intersection of different research fields. The Schwinger boson

representation of the VBS state (see (1.31)) relates to the Laughlin ansatz of the fractional quantum Hall effect [4, 26, 29]. The Laughlin wave function of the fractional quantum Hall effect is the VBS state on the complete graph [24]. The VBS state illustrates ground state properties of anti-ferromagnetic integer-spin chains with a Haldane gap [23]. In 1-dimension, the VBS state is related to the matrix product state and deformed VBS-models were studied in [37]. The theory of VBS state was generalized to the finitely correlated states and essentially developed [14, 15]. In 1-dimension, the correlation functions were obtained and studied in [15]. The entanglement of formation in VBS state was estimated in [40]. It has been showed that the VBS state can be used as a resource state in measurement-based quantum computation instead of the cluster state [7]. It was proved in [48] that VBS state allows universal quantum computation and an implementation of the AKLT Hamiltonian in optical lattices [19] has also been proposed.

This chapter introduces some of the main results on quantum entanglement in VBS states defined on a lattice or graph. We take a pedagogical approach, starting with the basics of the AKLT model, construction of VBS states and measures of entanglement. We shall consider a part (subsystem) of the system, *i.e.* a block of spins. It is described completely by the reduced density matrix of the block, which we call *the density matrix* later for short. The density matrix has been studied extensively. It contains information of all correlation functions [4, 31, 32, 50]. The entanglement properties of the VBS states has been studied by means of the density matrix as in [10–12, 18, 32, 36, 49–52].

The chapter is divided into seven sections including a complete treatment of 1-dimensional models:

1. A brief introduction to the topic. (§ 1.1)

2. The construction of the general AKLT Hamiltonian, introduction of the VBS ground state, and definition of different versions of the AKLT model: 1) The *basic* model; 2) The *generalized* (including the inhomogeneous) model. Proof of the uniqueness of the VBS ground state. (§ 1.2)

3. The concept of quantum entanglement, introduction of the subsystem, definition of the subsystem Hamiltonian and general properties of the density matrix for the model defined on a graph or a lattice. Proof of the relation between the non-zero spectrum of the density matrix and the degenerate ground states of the block Hamiltonian. (§ 1.3)

4. The simplest 1-dimensional basic model with spin-1. Calculation and diagonalization of the density matrix in an algebraic approach. Discussion

of the entanglement entropies. (§ 1.4)

5. The 1-dimensional homogeneous model with spin-S. Calculation and diagonalization of the density matrix using the Schwinger representation. Discussion of the entanglement entropies. Derivation of the relation between the density matrix and correlation functions. (§ 1.5)

6. The 1-dimensional inhomogeneous model treated in parallel with the homogeneous model. (§ 1.6)

7. Summary including some open problems. Conjecture on the density matrix and entropies in the large block limit. (§ 1.7)

1.2 The General AKLT Model

In the following we give the most general AKLT Hamiltonian and VBS states. The definition applies to both graphs and arbitrary lattices.

1.2.1 The Hamiltonian

The original AKLT Hamiltonian describes a spin interacting system, in which spins sitting at lattice sites interact with nearest neighbors. One of the most simple versions is an (1-dimensional) open chain of N sites with spin-1 at each site, and the Hamiltonian is given by [1]

$$H = \frac{1}{2}\sum_{j=0}^{N-1}\left(\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1} + \frac{1}{3}(\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1})^2 + \frac{2}{3}\right) \tag{1.1}$$

This Hamiltonian (1.1) looks like the Heisenberg Hamiltonian with an extra quadratic term (the proportionality factor 1/2 and the additive constant 2/3 are sometimes neglected which only shifts and scales the energy spectrum as a whole), but the physical system behaves quite differently. It was later generalized that the spin $\boldsymbol{S}_j$ at each site can take higher spin values or different values at different site, and one could apply different boundary conditions (*e.g.* a periodic boundary condition or an open boundary condition). An arbitrary boundary condition or distribution of spin values over sites may not yield a unique ground state (*e.g.* Hamiltonian (1.1) has 4-fold degenerate ground states), and we could find the condition for the existence of a uniqueness ground state (see § 1.2.5 and [36]). The Hamiltonian can be defined on higher dimensional lattices (*e.g.* 2-dimensional square or hexagonal lattice [1, 2]) or

an arbitrary graph (in that case we need to specify the meaning of a *nearest neighbor*). All these different variations share two common features:

1. The Hamiltonian is a collection of terms with only nearest neighbor interactions. *i.e.*

$$H = \sum_{\langle kl \rangle} H(k,l). \tag{1.2}$$

Here the Hamiltonian density $H(k,l)$ describes the interaction between spins at lattice sites or vertices (for a graph) k and l. Only nearest neighbor pairs $\langle kl \rangle$'s called *bonds* are involved in the sum in (1.2).

2. The Hamiltonian density $H(k,l)$ is a sum of terms with each term proportional to a projector. The proportionality coefficients are all positive. *i.e.*

$$H(k,l) = \sum_{J} C_J(k,l)\pi_J(k,l). \tag{1.3}$$

Here $\pi_J(k,l)$'s are projectors and $C_J(k,l)$'s are positive coefficients. Note that they may depend on the pair $\langle kl \rangle$ and the *bond spin* value labeled by J (The bound spin is defined as $\boldsymbol{J}_{kl} = \boldsymbol{S}_k + \boldsymbol{S}_l$). The meaning is this: The spin $\boldsymbol{S}_k$ with spin value S_k at site (or vertex) k is a $(2S_k + 1)$-dimensional representation of the $SU(2)$ Lie algebra, while $\boldsymbol{S}_l$ is a $(2S_l + 1)$-dimensional representation. The direct product of these two representations is reducible to a direct sum of irreducible representations with dimensions $2J + 1$ and J runs from $|S_k - S_l|$ to $S_k + S_l$. The Hilbert space 'splits' into these invariant subspaces labeled by J which is called the *bond spin* value of $\boldsymbol{S}_k$ and $\boldsymbol{S}_l$. (The eigenvalues of the Casimir operator – the square of the bond spin $(\boldsymbol{S}_k + \boldsymbol{S}_l)^2$ is $J(J+1)$.) The projector $\pi_J(k,l)$ projects on the invariant subspace with bond spin J. If we choose an orthonormal basis $\{|J,m\rangle \mid m = -J, \ldots, J\}$ for the subspace, such that $(\boldsymbol{S}_k + \boldsymbol{S}_l)^2|J,m\rangle = J(J+1)|J,m\rangle$ and $(S_k^z + S_l^z)|J,m\rangle = m|J,m\rangle$, then the projector could be written as

$$\pi_J(k,l) = \sum_{m=-J}^{J} |J,m\rangle\langle J,m|. \tag{1.4}$$

This form (1.4) is cumbersome in practical use and it is preferred to express the projector $\pi_J(k,l)$ explicitly in terms of spin operators $\boldsymbol{S}_k$ and $\boldsymbol{S}_l$. We shall do that in the next section (§ 1.2.2).

Even without an explicit form of the projectors, an immediate consequence of these two properties is that the Hamiltonian is *positive semi-definite*. [1] Furthermore, because of this, if we could construct a state $|\psi\rangle$ which has no projection on any of the specified bond spin-J states appearing in (1.3) for each bond, *i.e.* $\pi_J(k,l)|\psi\rangle = 0$, $\forall\ \langle kl\rangle$, then it has to be a ground state (with energy equal to zero) regardless of the specific values of the coefficients. [2]

1.2.2 The Projector

In order to complete the definition of the general AKLT Hamiltonian (1.2) and Hamiltonian density (1.3), we have to give an explicit expression of the projector $\pi_J(k,l)$ in terms of spin operators $\boldsymbol{S}_k$ and $\boldsymbol{S}_l$. There are two different approaches. The forms of $\pi_J(k,l)$ for a specific model such as the expression (1.1) or those for 1-dimensional models in § 1.4 , § 1.5 and § 1.6 can be obtained through either approach as follows.

1. The following two sets of operators, namely, the projectors

$$\{\pi_J(k,l) \mid J = |S_k - S_l|, \ldots, S_k + S_l\} \tag{1.5}$$

and the powers of the inner product $(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)$

$$\{(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)^n \mid n = 0, \ldots, 2S_<\}, \qquad S_< \equiv \min\{S_k, S_l\} \tag{1.6}$$

are both complete set of operators. One set is expressible in terms of the other. In other words, they are related by a linear transform:

$$\begin{aligned} & (\boldsymbol{S}_k \cdot \boldsymbol{S}_l)^n \\ = & \left(\frac{1}{2}\right)^n \left[(\boldsymbol{S}_k + \boldsymbol{S}_l)^2 - S_k(S_k+1) - S_l(S_l+1)\right]^n \sum_{J=|S_k-S_l|}^{S_k+S_l} \pi_J(k,l) \\ = & \sum_{J=|S_k-S_l|}^{S_k+S_l} \left(\frac{1}{2}\right)^n \left[J(J+1) - S_k(S_k+1) - S_l(S_l+1)\right]^n \pi_J(k,l) \end{aligned} \tag{1.7}$$

[1] The Hamiltonian is essentially a sum of projectors with positive coefficients. A projector π satisfies $\pi^2 = \pi$. So that for an arbitrary state $|\psi\rangle$, we have $\langle\psi|\pi|\psi\rangle = \langle\psi|\pi^2|\psi\rangle = (\pi|\psi\rangle, \pi|\psi\rangle) \geq 0$, in which $(*\ , *)$ denotes an inner product.

[2] Some authors add or omit additive constants in the expression of projectors. *e.g.* in (1.1) the constant 2/3 can be dropped. This may shift the ground state energy but does not affect the form of the ground state because the ground state is constructed to have no projection on the specified subspaces for every bond.

for $n = 0, \ldots, 2S_<$. In (1.7) we have used

$$\sum_{J=|S_k-S_l|}^{S_k+S_l} \pi_J(k,l) = I \tag{1.8}$$

being the identity. This set of $2S_< + 1$ linear equations (1.7) can be inverted, which express the projector $\pi_J(k,l)$ as a polynomial of the inner product $(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)$.

2. Another approach is to realize that if an operator $\mathcal{P}(k,l)$ satisfies the following condition

$$\mathcal{P}(k,l)\pi_{J'}(k,l) = \delta_{JJ'}\pi_J(k,l), \qquad \forall\ J' \tag{1.9}$$

then the operator $\mathcal{P}(k,l)$ is identified with $\pi_J(k,l)$ because

$$\begin{aligned} \mathcal{P}(k,l) &= \mathcal{P}(k,l) \sum_{J'=|S_k-S_l|}^{S_k+S_l} \pi_{J'}(k,l) \\ &= \left(\sum_{J'=|S_k-S_l|}^{S_k+S_l} \delta_{JJ'} \right) \pi_J(k,l) = \pi_J(k,l). \end{aligned} \tag{1.10}$$

Therefore we could construct an operator satisfying the condition (1.9):

$$\mathcal{P}(k,l) = \prod_{|S_k-S_l|\le j\le S_k+S_l}^{j\neq J} \frac{(\boldsymbol{S}_k + \boldsymbol{S}_l)^2 - j(j+1)}{J(J+1) - j(j+1)}. \tag{1.11}$$

When $\mathcal{P}(k,l)$ acting on $\pi_{J'}(k,l)$, we have:

(a) If $J' \neq J$, then the numerator of one factor in the product vanishes, so that $\mathcal{P}$ vanishes;

(b) If $J' = J$, all factors in the product become equal to 1, so as the expression $\mathcal{P}$.

So that (1.11) is the projector $\pi_J(k,l)$. Operator $\pi_J(k,l) = \mathcal{P}(k,l)$ in (1.11) projects the bond spin $\boldsymbol{J}_{kl} \equiv \boldsymbol{S}_k + \boldsymbol{S}_l$ on the subspace with fixed total spin value J and $|S_k - S_l| \le J \le S_k + S_l$. Note that we could expand $(\boldsymbol{S}_k + \boldsymbol{S}_l)^2 = 2\boldsymbol{S}_k \cdot \boldsymbol{S}_l + S_k(S_k+1) + S_l(S_l+1)$. Therefore projector $\pi_J(k,l)$ in (1.11) is a polynomial in the scalar product $(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)$ of degree $2S_<$, where $S_< \equiv \min\{S_k, S_l\}$ is the minimum of the two spin

values of the same bond $\langle kl \rangle$. For example with $S_k = S_l = 1$, we may have a quadratic polynomial as in (1.1):

$$\pi_2(k,l) = \frac{1}{6}(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)^2 + \frac{1}{2}(\boldsymbol{S}_k \cdot \boldsymbol{S}_l) + \frac{1}{3}. \tag{1.12}$$

1.2.3 The Basic AKLT Model

The Hamiltonian

Once we have the building blocks for the Hamiltonian from § 1.2.1 and § 1.2.2 , various types of the AKLT model can be constructed. Let us start with the definition of the *basic* AKLT model on a connected graph or lattice. (Any lattice is a special graph with periodic structure; our notations and definitions refer to the most general). A *graph* consists of two types of elements, namely *vertices* and *edges*. Every edge *connects* two vertices. As in Figure (1.1), a vertex is drawn as a (large) circle and an edge is drawn as a solid line connecting two vertices. For every pair of vertices in the *connected* graph, there is a *walk* [3] from one to the other. Vertices can also be called *sites* and edges sometimes called *links* or *bonds*. In a graph, a pair of vertices connected by an edge is regarded nearest neighbors, *i.e.* the terms edge, bond and nearest neighbor are equivalent and interchangeable. (For a lattice, vertices become sites and bonds become lattice vectors connecting nearest neighboring sites.) In the case of a disconnected graph, the Hamiltonian (1.2) is a direct sum with respect to connected components and the ground state is a direct product. Therefore we shall need only to study a connected graph. Also, assuming that the graph consists of more than one vertices to avoid the trivial case where there would be no interaction at all.

Let us introduce mathematical notations. By $\boldsymbol{S}_l$ we shall denote the spin operator located at vertex l with spin value S_l. In the *basic* model we require that $S_l = \frac{1}{2}z_l$, where z_l is the number of incident edges connected to vertex l, also known as the *valence* or *coordination number* (the number of nearest neighbors of the vertex l). The relation between the spin value and coordination number must be true for any vertex l, including boundaries. This will guarantee the uniqueness of the ground state, see § 1.2.5 . For a lattice, this condition would also yield that bulk spins (spins not on the boundary) take the same value $\frac{1}{2}z$ because the number of nearest neighbors z is a constant.

In the *basic* model we define the Hamiltonian density $H(k,l)$ for bond

[3] A *walk* is an alternating sequence of vertices and edges, beginning and ending with a vertex, in which each vertex is incident to the two edges that precede and follow it in the sequence, and the vertices that precede and follow an edge are the endvertices of that edge.

(edge) $\langle kl \rangle$ as

$$H(k,l) = C(k,l)\ \pi_{S_k+S_l}(k,l), \qquad H(k,l) \geq 0 \tag{1.13}$$

with $C(k,l)$ an arbitrary positive real coefficient (it may depend on the bond $\langle kl \rangle$). So that the Hamiltonian density for each bond (edge) is proportional to the projector on the subspace with the highest possible bond spin value $(S_k + S_l)$. The physical meaning is that interacting spins do not form the highest possible bond spin (this will increase the energy) in the ground state. Then the Hamiltonian according to (1.2) is

$$H = \sum_{\langle kl \rangle} H(k,l) = \sum_{\langle kl \rangle} C(k,l)\pi_{S_k+S_l}(k,l). \tag{1.14}$$

Here we sum over all bonds (edges) $\langle kl \rangle$. Note that for a lattice all the highest bond spin values for bulk spins are the same and equal to half the coordination number $z/2$. For example, the basic model defined on a 2-dimensional square lattice must have spin-2 in the bulk and π_4 in the Hamiltonian; also, the Hexagonal lattice has spin-3/2 and π_3.

The VBS State – Graphical Method

The Hamiltonian (1.14) with condition

$$S_l = \frac{1}{2} z_l \tag{1.15}$$

has a unique ground state [1, 2, 4, 36] known as the Valence-Bond-Solid (VBS) state. It can be constructed in a graphical way as follows (see Figure 1.1). Each vertex l is represented by z_l spin-$\frac{1}{2}$'s. We associate each spin-$\frac{1}{2}$ with an incident edge. In such a way each edge has two spin-$\frac{1}{2}$'s at its ends. We anti-symmetrize the spin states of these two spin-$\frac{1}{2}$'s. So that anti-symmetrization is done along each edge. These anti-symmetrizations ensure that there is no projection on the highest bond spin states for every bond. Then we also symmetrize the product of spin-$\frac{1}{2}$'s at each vertex (each large circle in Figure 1.1). These symmetrizations preserve the correct spin value at each vertex.

Let us write down the VBS ground state algebraically following this approach. We label the particular dot from vertex l connected with some dot from vertex k by l_k (correspondingly, that dot from vertex k is labeled by k_l). In this way we have specified a unique prescription of indices with dots. Then

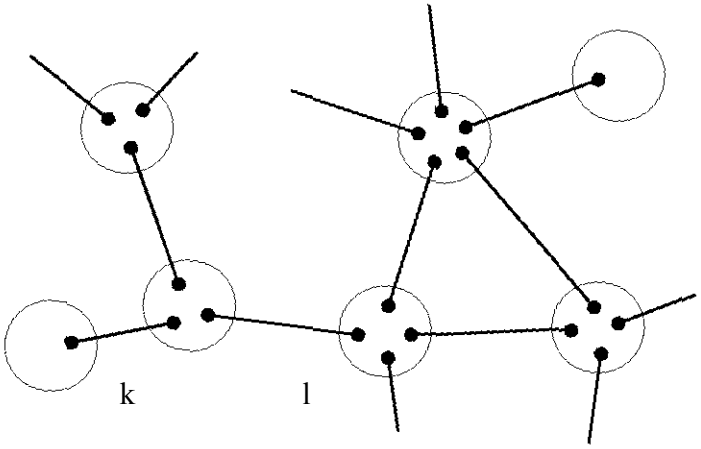

Figure 1.1: Example of a part of the graph including vertex k with $z_k = 3$ and vertex l with $z_l = 4$. Black dots represent spin-$\frac{1}{2}$ states, which are enclosed by large circles representing vertices and symmetrization of the product of spin-$\frac{1}{2}$'s at each vertex. Solid lines represent edges (bonds) which anti-symmetrize the pair of connected spin-$\frac{1}{2}$'s.

the anti-symmetrization results in the singlet state

$$|\Phi\rangle_{kl} = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{l_k} |\downarrow\rangle_{k_l} - |\downarrow\rangle_{l_k} |\uparrow\rangle_{k_l} \right), \tag{1.16}$$

where $|\uparrow\rangle$ (or $|\downarrow\rangle$) denotes spin up (or down) states referring to a basis. The direct product of all these $|\Phi\rangle$ singlet states corresponds to all edges (bonds) in our Figure 1.1:

$$\prod_{\langle kl \rangle} |\Phi\rangle_{kl}. \tag{1.17}$$

We still have to complete the symmetrization (circles) at each vertex. We denote the symmetrization operator of z_l black dots in vertex l by $\mathbf{P}(l)$. The action of $\mathbf{P}(l)$ on any product of z_l spin-$\frac{1}{2}$'s is

$$\begin{aligned} & \mathbf{P}(l) |\chi_{l_{k_1}}\rangle_{l_{k_1}} |\chi_{l_{k_2}}\rangle_{l_{k_2}} \cdots |\chi_{l_{k_{z_l}}}\rangle_{l_{k_{z_l}}} \qquad (1.18) \\ = & \sum_{\sigma}^{z_l! \text{ terms}} |\chi_{l_{k_{\sigma(1)}}}\rangle_{l_{k_1}} |\chi_{l_{k_{\sigma(2)}}}\rangle_{l_{k_2}} \cdots |\chi_{l_{k_{\sigma(z_l)}}}\rangle_{l_{k_{z_l}}}, \qquad \chi = \uparrow \text{ or } \downarrow \end{aligned}$$

where $k_1, k_2, \ldots, k_{z_l}$ are the z_l spin-$\frac{1}{2}$'s (block dots) belonging to vertex l (the index also refers to the z_l vertices connected to vertex l by an edge) and σ is a permutation of the indices:

$$\sigma = \begin{pmatrix} 1 & 2 & \cdots & z_l \\ \sigma(1) & \sigma(2) & \cdots & \sigma(z_l) \end{pmatrix}. \tag{1.19}$$

All permutations are summed up in (1.18). Then the symmetrization at each vertex is carried out by taking the product $\prod_l \mathbf{P}(l)$ of all vertices. Finally, the unique VBS ground state can be written as

$$|\text{VBS}\rangle = \prod_l \mathbf{P}(l) \prod_{\langle kl \rangle} |\Phi\rangle_{kl}. \tag{1.20}$$

Here the first product runs over all vertices and the second over all edges (bonds). Note that the VBS state in (1.20) is not normalized in general. If the coordination number z_l is a constant over all vertices in the graph except for boundaries (such as in the case of a lattice), then we would have the same spin value at each bulk vertex. In that case the *basic* model is also referred to as the *homogeneous* model.

1.2.4 The Generalized AKLT Model

The Hamiltonian

In the *generalized* AKLT model, relation (1.15) is generalized. We associate a positive integer M_{kl} ($M_{kl} \equiv M_{lk}$) to each edge $\langle kl \rangle$ of the graph (or each bond of a lattice). We shall call M_{kl} *multiplicity numbers*. Similar to the basic model, the Hamiltonian describes interactions between nearest neighbors (vertices connected by an edge):

$$H = \sum_{\langle kl \rangle} H(k,l). \tag{1.21}$$

However, the Hamiltonian density is no longer proportional to a single projector as in (1.13) in general. Instead, it is a linear combination of projectors

$$H(k,l) = \sum_{J=S_k+S_l-M_{kl}+1}^{S_k+S_l} C_J(k,l)\ \pi_J(k,l), \tag{1.22}$$
$$1 \le M_{kl} \le 2S_< \equiv \min\{S_k, S_l\}.$$

Projector $\pi_J(k,l)$ is given by (1.11), and $C_J(k,l)$'s are arbitrary positive coefficients. So that $H(k,l)$ projects the bond spin on the subspace with bond spin value J greater than $S_k + S_l - M_{kl}$. Physically formation of any bond spin higher than $S_k + S_l - M_{kl}$ would increase the energy.

The condition of uniqueness of the ground state was introduced in [36]:

$$2S_l = \sum_k M_{kl}, \qquad \forall\ l. \tag{1.23}$$

Here S_l is the spin value at vertex l and we sum over all edges incident to vertex l (connected to vertex l). The Hamiltonian (1.21) has a unique ground state if (1.23) is valid, see § 1.2.5 . The relation $2S_l = z_l$ for the *basic* model is a special case when all $M_{kl} = 1$. Also, when $M_{kl} = 1$, the Hamiltonian density (1.22) reduces to that of the basic model (1.13). The condition (1.23) can be put into an invariant form. Let us define a column vector $\mathbf{S}$, the l^{th} component of which is associated with vertex l of the graph and equal to S_l. The number of components is equal to the number of vertices N in the whole graph. Next, we define another column vector $\mathbf{M}$ with its dimension equal to the number of edges M in the graph. The k^{th} and l^{th} components of this vector are associated with edge $\langle kl \rangle$ and both equal to M_{kl}. The most important geometrical characteristic of the graph is the vertex-edge incidence matrix $\hat{\mathbf{I}}$ (see [27]). This is a rectangular matrix with N rows and M columns. Each row is associated with the vertex and each column is associated with the edge. If the vertex belongs to the edge the corresponding matrix element is equal to one, otherwise zero. Then the condition (1.23) of uniqueness can be re-written as

$$2\ \mathbf{S} = \hat{\mathbf{I}} \cdot \mathbf{M}. \tag{1.24}$$

For more details we refer to [36].

The VBS State – Schwinger Representation

Under condition (1.23) or (1.24), the unique ground state of Hamiltonian (1.21) is referred to as the generalized VBS state. It is constructed by introducing the Schwinger boson representation [4, 18, 32, 36, 50–52]. This method uses a pair of bosonic creation and annihilation operators (similar to the treatment of the harmonic oscillator problem) to realize the $SU(2)$ Lie algebra.

Define a pair of independent canonical bosonic operators a_l and b_l for each vertex (or site) l:

$$[\ a_k\ ,\ a_l^\dagger\ ] = [\ b_k\ ,\ b_l^\dagger\ ] = \delta_{kl} \tag{1.25}$$

with all other commutators vanishing:

$$[\ a_k\ ,\ a_l\ ] = [\ b_k\ ,\ b_l\ ] = [\ a_k\ ,\ b_l\ ] = [\ a_k\ ,\ b_l^\dagger\ ] = 0, \qquad \forall\ k, l. \tag{1.26}$$

Spin operators are represented as

$$S_l^+ = a_l^\dagger b_l, \qquad S_l^- = b_l^\dagger a_l, \qquad S_l^z = \frac{1}{2}(a_l^\dagger a_l - b_l^\dagger b_l). \tag{1.27}$$

It is straightforward to verify that the $SU(2)$ Lie algebra is realized. To reproduce the dimension of the spin-S_l Hilbert space at vertex l, a constraint on the total boson occupation number is required:

$$\hat{S}_l \equiv \frac{1}{2}(a_l^\dagger a_l + b_l^\dagger b_l) = S_l. \tag{1.28}$$

i.e. any physical spin state $|\psi\rangle_l$ at vertex l must satisfy $\hat{S}_l|\psi\rangle_l = S_l|\psi\rangle_l$. In this framework the spin state $|S_l, m_l\rangle_l$ such that $\boldsymbol{S}_l^2|S_l, m_l\rangle_l = S_l(S_l+1)|S_l, m_l\rangle_l$ and $S_l^z|S_l, m_l\rangle_l = m_l|S_l, m_l\rangle_l$ is represented by

$$|S_l, m_l\rangle_l = \frac{(a_l^\dagger)^{S_l+m_l}(b_l^\dagger)^{S_l-m_l}}{\sqrt{(S_l+m_l)!(S_l-m_l)!}}|\text{vac}\rangle_l, \tag{1.29}$$

where the *vacuum* $|\text{vac}\rangle_l$ is annihilated by any of the annihilation operators:

$$a_l\,|\text{vac}\rangle_l = b_l\,|\text{vac}\rangle_l = 0. \tag{1.30}$$

As a result, the VBS ground state in the Schwinger representation is constructed as

$$|\text{VBS}\rangle = \prod_{\langle kl\rangle}\left(a_k^\dagger b_l^\dagger - b_k^\dagger a_l^\dagger\right)^{M_{kl}}|\text{vac}\rangle. \tag{1.31}$$

It worth mentioning that this representation shows that for a full graph (each vertex is connected to every other vertex by definition) the VBS state coincides with the Laughlin wave function [4, 24, 26]. In (1.31) the product runs over all bonds (edges) and the vacuum $|\text{vac}\rangle$ is the direct product of vacuums of each vertex

$$|\text{vac}\rangle = \bigotimes_l |\text{vac}\rangle_l, \tag{1.32}$$

which is destroyed by any annihilation operators a_l or b_l, $\forall\ l$. (Note that

$[\, a_k^\dagger \,,\, b_l^\dagger \,] = 0, \forall\, k, l.)$

To prove that (1.31) is the ground state we need only to verify for any vertex l and bond (edge) $\langle kl \rangle$:

1. The total power of $a_l^\dagger$ and $b_l^\dagger$ is $2S_l$, so that we have spin-S_l at vertex l;

2. The z-component of the bond spin satisfies

$$-\frac{1}{2}(\sum_{l' \neq l} M_{l'k} + \sum_{k' \neq k} M_{k'l}) \leq J_{kl}^z \equiv S_k^z + S_l^z \leq \frac{1}{2}(\sum_{l' \neq l} M_{l'k} + \sum_{k' \neq k} M_{k'l}) \tag{1.33}$$

by a binomial expansion. Consequently, the maximum value of the bond spin J_{kl} is $\frac{1}{2}(\sum_{l' \neq l} M_{l'k} + \sum_{k' \neq k} M_{k'l}) = S_k + S_l - M_{kl}$ (from $SU(2)$ invariance, see § 1.5.8 and [4]).

Therefore, the state $|\text{VBS}\rangle$ defined in (1.31) has spin-S_l at vertex l and no projection onto the $J_{kl} > S_k + S_l - M_{kl}$ subspace for any bond (edge). The introduction of Schwinger bosons can be used to construct a spin coherent state basis (as expected due to the similarity with the harmonic oscillator) in which spins at each vertex behave as classical unit vectors, see § 1.5.1 and [18, 32, 36, 50, 51]. The coherent state basis converts algebraic computations into classical integrals which becomes extremely useful in later sections.

1.2.5 The Uniqueness Condition

As stated in previous sections, the condition for the existence of a unique VBS ground state is $2S_l = z_l$ for the basic model and $2S_l = \sum_k M_{kl}$ for the generalized model (the former being a special case of the latter). In this section we prove the uniqueness condition, *i.e.* the equation

$$H|\Psi\rangle = 0 \tag{1.34}$$

with H the AKLT Hamiltonian (1.21) has exactly one solution under the condition (1.23) or (1.24). Note that this expression (1.34) is equivalent to

$$\pi_J(k,l)|\Psi\rangle = 0, \qquad \forall\, \langle k,l \rangle, \qquad S_k + S_l - M_{kl} + 1 \leq J \leq S_k + S_l \tag{1.35}$$

because of the positive semi-definiteness of every projector π_J and the positive coefficients C_J.

In order to prove the uniqueness condition, we first prove the following lemma.

Lemma 1.1
All solutions of the equation

$$\pi_J(k,l)|\psi\rangle = 0, \qquad S_k + S_l - M_{kl} + 1 \leq J \leq S_k + S_l \tag{1.36}$$

for fixed k and l can be represented in the following form

$$|\psi\rangle = f(a^\dagger, b^\dagger)(a_k^\dagger b_l^\dagger - a_l^\dagger b_k^\dagger)^{M_{kl}}|\text{vac}\rangle. \tag{1.37}$$

Here $f(a^\dagger, b^\dagger)$ is some polynomial in $a_k^\dagger$, $b_k^\dagger$ and $a_l^\dagger$, $b_l^\dagger$. For convenience, let us apply the Weyl representation of the $SU(2)$ Lie algebra. Consider the space of polynomials in pairs of variables x_l and y_l with coefficients in $\mathbf{C}$. We represent operator $a_l^\dagger$ as multiplication on x_l and $b_l^\dagger$ as multiplication on y_l. At site l we have

$$\begin{aligned} S_l^+ &= x_l \frac{\partial}{\partial y_l}, & S_l^- &= y_l \frac{\partial}{\partial x_l} \\ 2S_l^z &= x_l \frac{\partial}{\partial x_l} - y_l \frac{\partial}{\partial y_l}, & 2\hat{S}_l &= x_l \frac{\partial}{\partial x_l} + y_l \frac{\partial}{\partial y_l}. \end{aligned} \tag{1.38}$$

A basis of the $(2S_l + 1)$-dimensional irreducible representation of spin-S_l can be chosen in such a way:

$$\mathbf{V}_{S_l} = \{x_l^{S_l+m_l} y_l^{S_l-m_l} \mid m = -S, \ldots, S\}. \tag{1.39}$$

These monomials with total power $2S_l$ are clearly eigenvectors of S_l^z and $\hat{S}_l$. Now let us consider the tensor product of two irreducible representations $\mathbf{V}_{S_l} \otimes \mathbf{V}_{S_k}$. Define the bond spin $\boldsymbol{J}_{kl} \equiv \boldsymbol{S}_k + \boldsymbol{S}_l$, then

$$\begin{aligned} J_{kl}^+ &= x_k \frac{\partial}{\partial y_k} + x_l \frac{\partial}{\partial y_l}, \\ J_{kl}^- &= y_k \frac{\partial}{\partial x_k} + y_l \frac{\partial}{\partial x_l}, \\ 2J_{kl}^z &= x_k \frac{\partial}{\partial x_k} + x_l \frac{\partial}{\partial x_l} - y_k \frac{\partial}{\partial y_k} - y_l \frac{\partial}{\partial y_l}, \\ 2\hat{J}_{kl} &= x_k \frac{\partial}{\partial x_k} + x_l \frac{\partial}{\partial x_l} + y_k \frac{\partial}{\partial y_k} + y_l \frac{\partial}{\partial y_l}. \end{aligned} \tag{1.40}$$

The tensor product of irreducible representation can be reduced to a direct

sum of irreducible representations

$$\mathbf{V}_{S_k} \otimes \mathbf{V}_{S_l} = \bigoplus_{J=|S_k-S_l|}^{S_k+S_l} \mathbf{V}_J. \tag{1.41}$$

Now we construct the highest vector (polynomial) v_J of irreducible representation $\mathbf{V}_J$ with fixed J:

$$J^+_{kl} v_J = 0, \qquad J^z_{kl} v_J = J v_J, \qquad \hat{J}_{kl} v_J = (S_k + S_l) v_J. \tag{1.42}$$

It must have a total power $2(S_k + S_l)$, so that the form can be taken as

$$v_J = \sum_{m_k+m_l=J} C_{m_k m_l} x_l^{S_l+m_l} y_l^{S_l-m_l} x_k^{S_k+m_k} y_k^{S_k-m_k}. \tag{1.43}$$

This form already satisfies the second and third equations in (1.42). After rearranging terms (relabeling indices), the first equation of (1.42) becomes

$$\begin{aligned} J^+_{kl} v_J \;\; = \;\; & \sum_{m_k=0}^{J-1} \left[(S_k - m_k) C_{m_k, J-m_k} + (S_l - J + m_k + 1) C_{m_k+1, J-m_k-1} \right] \\ & \cdot x_k^{S_k+m_k+1} y_k^{S_k-m_k-1} x_l^{S_l+J-m_k} y_l^{S_l-J+m_k}. \end{aligned} \tag{1.44}$$

Because of the linear independence of the monomials appearing in (1.44), the coefficients must vanish, which yields the following recurrence relation

$$C_{m_k+1, J-m_k-1} = -\frac{S_k - m_k}{S_l - J + m_k + 1} C_{m_k, J-m_k}. \tag{1.45}$$

The solution to (1.45) in terms of $C_{0,J}$ is

$$C_{m_k, J-m_k} = \frac{(-1)^{S_k-m_k} \begin{pmatrix} S_k + S_l - J \\ S_k - m_k \end{pmatrix}}{(-1)^{S_k} \begin{pmatrix} S_k + S_l - J \\ S_k \end{pmatrix}} C_{0,J}. \tag{1.46}$$

Therefore by substituting (1.46) into (1.43) and recognizing a binomial expan-

sion, the form of v_J is found to be

$$\begin{aligned} v_J &= \frac{C_{0,J}}{(-1)^{S_k}\begin{pmatrix} S_k+S_l-J \\ S_k \end{pmatrix}} x_k^{S_k-S_l+J} x_l^{S_l-S_k+J} (x_k y_l - x_l y_k)^{S_k+S_l-J} \\ &\propto x_k^{2S_k-M} x_l^{2S_l-M} (x_k y_l - x_l y_k)^M, \qquad M = S_k+S_l-J. \end{aligned} \tag{1.47}$$

The over all constant factor is irrelevant. All other vectors of representation $\mathbf{V}_J$ can be obtained from the highest vector v_J by applications of operator J_{kl}^-. Notice that J_{kl}^- commutes with the factor $(x_k y_l - x_l y_k)$

$$[\ J_{kl}^-\ ,\ x_k y_l - x_l y_k\ ] = 0. \tag{1.48}$$

So that all vectors of representation $\mathbf{V}_J$ are divisible by

$$(x_k y_l - x_l y_k)^M, \qquad M = S_k+S_l-J. \tag{1.49}$$

In other words, any vector (polynomial in x_k, y_k and x_l, y_l) in the vector space spanned by $\mathbf{V}_J$ has a common factor (1.49). As a consequence, if there is no projection on the states with bond spin values

$$S_k+S_l-M_{kl}+1 \le J \le S_k+S_l \tag{1.50}$$

after summation of spins $\boldsymbol{S}_k$ and $\boldsymbol{S}_l$ (*i.e.* no projection on $\mathbf{V}_J$ with $S_k+S_l-M_{kl}+1 \le J \le S_k+S_l$), then a factor

$$(x_k y_l - x_l y_k)^{M_{kl}} \tag{1.51}$$

can be isolated. *i.e.* Any vector in $\sum_{J=|S_k-S_l|}^{S_k+S_l-M_{kl}} \mathbf{V}_J$ would have a common factor (1.51). Moreover, this fact is independent of whether we are using the Weyl representation or the Schwinger representation of the Lie algebra. Therefore, any solution to (1.36) must take the form of (1.37) with the factor $(a_k^\dagger b_l^\dagger - a_l^\dagger b_k^\dagger)^{M_{kl}}$ isolated. Thus we have proved **Lemma 1.1**.

Now let us use **Lemma 1.1** to prove the uniqueness condition (1.23) or (1.24). Note that (1.36) is valid for each bond $\langle kl\rangle$, consequently any ground state $|\Psi\rangle$ of the Hamiltonian satisfying (1.34) and (1.35) can be presented in the form

$$|\Psi\rangle = \prod_{\langle kl\rangle} F(a^\dagger, b^\dagger)(a_k^\dagger b_l^\dagger - a_l^\dagger b_k^\dagger)^{M_{kl}}|\text{vac}\rangle, \tag{1.52}$$

where $F(a^\dagger, b^\dagger)$ is some polynomial in $a^\dagger$'s and $b^\dagger$'s. Now we have to make sure

that in (1.52) each vertex (site) should have the correct spin value. By applying $2\hat{S}_l = (a_l^\dagger a_l + b_l^\dagger b_l)$ to the state $|\Psi\rangle$, we realize that the explicit factor in (1.52) contribute to $2S_l$ (denoting the eigenvalue of $2\hat{S}_l$) exactly the value $\sum_{\langle kl\rangle} M_{kl}$ which is the sum of powers of $a_l^\dagger$ and $b_l^\dagger$. A comparison with expression (1.23) or (1.24) shows that if we require this condition $2S_l = \sum_{\langle kl\rangle} M_{kl}$, then each site would already have the correct spin value with the presence in (1.52) of the explicit factor only. Therefore the degree of the polynomial in variables $a_l^\dagger$ and $b_l^\dagger$ is zero. This is true for every site l. Therefore the polynomial $F(a^\dagger, b^\dagger)$ is a constant which can be removed. So that we have proved that the uniqueness condition (1.23) or (1.24) guarantees the existence (through explicit construction in § 1.2.4) and uniqueness of an energy ground state – the VBS state.

1.3 The Subsystem and Measures of Entanglement

The VBS states constructed in previous sections § 1.2.3 and § 1.2.4 as ground states of AKLT models are highly entangled states. The quantification of entanglement is our main subject of study.

1.3.1 The Block Density Matrix and the Block Hamiltonian

The Block Density Matrix and Entropies

The VBS state (see (1.20) and (1.31)) has non-trivial entanglement properties. The density matrix of the VBS state is a projector (a pure state density matrix):

$$\boldsymbol{\rho} = \frac{|\mathrm{VBS}\rangle\langle\mathrm{VBS}|}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle}. \tag{1.53}$$

In order to analyze the entanglement, let us cut the original graph (lattice) into two subgraphs (sublattices) B and E. That is, we cut through some number of edges (bonds) such that the resulting graph (or lattice) $B \cup E$ is disconnected (no edge (bond) between B and E). We may call one of them, say B, the *block*, and the other one E the *environment*. The distinction is arbitrary and the two subsystems are equivalent in measuring entanglement.

Let us focus on the block (subsystem B). It is described by the density matrix $\boldsymbol{\rho}_B$ of the block (obtained by tracing out all degrees of freedom of the

environment E from the density matrix $\boldsymbol{\rho}$ (1.53)):

$$\boldsymbol{\rho}_B = \mathrm{tr}_E \left[\, \boldsymbol{\rho} \, \right]. \tag{1.54}$$

In (1.54) and below we use subscript B for *block* and E for *environment*. After tracing out all degrees of freedom outside the block the density matrix $\boldsymbol{\rho}_B$ is, in general, a mixed state density matrix (unless the pure state density matrix $\boldsymbol{\rho}$ of the whole system projects on a product state, which is obviously not our case of the VBS state). Formula (1.54) is the definition of the block (subsystem) density matrix and it satisfies all three requirements of a density matrix:

1. The trace $\mathrm{tr}_B \left[\, \boldsymbol{\rho}_B \, \right] = 1$ and hermiticity $\boldsymbol{\rho}_B^\dagger = \boldsymbol{\rho}_B$ follow immediately from those of $\boldsymbol{\rho}$;

2. The positive semi-definiteness is seen by picking up an arbitrary state $|\psi\rangle_B$ of the block and realizing that

$$\begin{aligned} {}_B\langle\psi|\boldsymbol{\rho}_B|\psi\rangle_B &= \mathrm{tr}_B \left[\, \boldsymbol{\rho}_B |\psi\rangle_B\langle\psi| \, \right] \\ &= \mathrm{tr}_B \left[\, (\mathrm{tr}_E \boldsymbol{\rho})|\psi\rangle_B\langle\psi| \, \right] \\ &= \mathrm{tr} \left[\, \boldsymbol{\rho}|\psi\rangle_B\langle\psi| \otimes I_E \, \right] \geq 0, \end{aligned} \tag{1.55}$$

   because of the positive semi-definiteness of $\boldsymbol{\rho}$ (I_E is the identity of the environment).

The density matrix $\boldsymbol{\rho}_B$ is a central quantity in description of the subsystem (block). It contains all correlation functions in the VBS ground state as matrix entries [4, 31, 32, 50]. (The relation between elements of the density matrix and correlation functions is given in § 1.5.9 .) It is essential in measuring the entanglement which is our main subject.

The entanglement can be measured or *quantified* by the von Neumann entropy

$$S_{\mathrm{v\ N}} = -\mathrm{tr_B} \left[\, \boldsymbol{\rho}_B \ln \boldsymbol{\rho}_B \, \right] = -\sum_{\lambda \neq 0} \lambda \ln \lambda \tag{1.56}$$

or the Rényi entropy

$$S_{\mathrm{R}}(\alpha) = \frac{1}{1-\alpha} \ln \left\{ \mathrm{tr}_B \left[\, \boldsymbol{\rho}_B^\alpha \, \right] \right\} = \frac{1}{1-\alpha} \ln \left(\sum_{\lambda \neq 0} \lambda^\alpha \right), \qquad \alpha > 0. \tag{1.57}$$

Here λ's are (non-zero) eigenvalues of the density matrix $\boldsymbol{\rho}_B$ and α is an arbitrary parameter. Note that the Rényi entropy can be regarded a generalization

of the von Neumann entropy and reduces to the latter in the limit $\alpha \to 1$. The von Neumann entropy is a proper extension of the Gibbs entropy (in statistical mechanics) and the Shannon entropy (in information theory) to the quantum case. (The Shannon entropy measures the uncertainty associated with a classical probability distribution. Whereas in quantum case a density operator replaces a classical distribution.) It was shown by using the Schmidt decomposition (Section 2.5 of [41]) that non-zero eigenvalues of the density matrix of subsystem B (block) is equal to those of the density matrix of subsystem E (environment). So that the two subsystems are equivalent in measuring entanglement in terms of entanglement entropies, *i.e.* $S_{\mathrm{v\ N}}[B] = S_{\mathrm{v\ N}}[E]$ and $S_{\mathrm{R}}[B] = S_{\mathrm{R}}[E]$. This fact has been used in obtaining entanglement entropies of 1-dimensional VBS states as in [11, 32] instead of diagonalizing the density matrix directly. We will study the entropies in detail in following sections.

The Block Hamiltonian

The AKLT block density matrix $\boldsymbol{\rho}_B$ possesses certain characteristic properties which distinguish the VBS states from others. We shall show in § 1.3.3 that the spectrum of the density matrix $\boldsymbol{\rho}_B$ contains a lot of zero eigenvalues. In order to understand this and give the subsystem (block) a more complete description, we first introduce the Hamiltonian of the subsystem (called the *block* Hamiltonian).

The *block* Hamiltonian H_B is the sum of Hamiltonian densities $H(k,l)$ with both $k \in B$ and $l \in B$, *i.e.* nearest neighbor interactions (bond terms) within the block B:

$$H_B = \sum_{\langle kl\rangle \in B} H(k,l), \qquad k \in B, \quad l \in B. \tag{1.58}$$

Here $H(k,l)$ is given in (1.13) for the basic model and (1.22) for the generalized model, for k and l connected by an edge (bond). In (1.58) no cut edges are present (boundary edges between subgraphs B and E removed). In other words, the block Hamiltonian is the *internal* interactions of the subsystem B. This Hamiltonian has degenerate ground states because uniqueness conditions (1.15) and (1.23) are no longer valid.

Let us discuss the degeneracy of ground states of (1.58). Let us denote by $N_{\partial B}$ the number of vertices on the boundary ∂B of the block B. The boundary consists of those vertices (sites) with one or more cut incident edge (bond), see Figure 1.2. The degeneracy *deg* of ground states of H_B is given by the

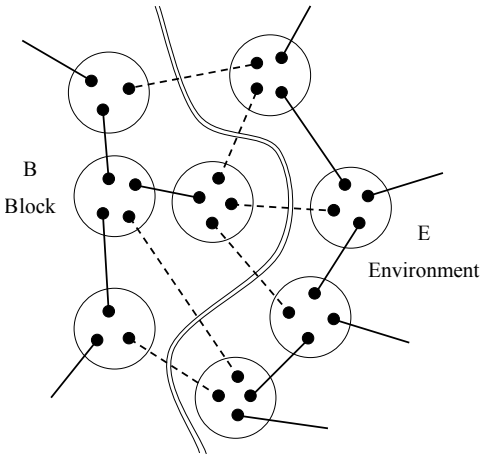

Figure 1.2: Example of the cutting for the basic model. The curved double line represents the boundary between the two subgraphs. We have the block B on the left and the environment E on the right. Solid lines represent edges (bonds) while dashed lines represent cut edges (cut bonds). Each dashed line connects two dots. All vertices in the figure belong to the boundary of B or E because of the presence of one or more cut incident edges (dashed lines).

Katsura's formula

$$deg = \prod_{l\in\partial B}\left[\left(\sum_{k\in\partial E} M_{kl}\right)+1\right], \qquad \langle kl\rangle \in \{\text{cut edges}\}. \tag{1.59}$$

Here ∂B denotes vertices (sites) on the boundary of the block B and ∂E are vertices (sites) on the boundary of the environment E. In (1.59) we have $N_{\partial B}$ terms in the product. Formula (1.59) is valid for both the basic and the generalized model. For the basic model all $M_{kl} = 1$, including those corresponding to cut edges. Take, for example, a particularly simple case that each vertex on the boundary of the block ∂B was connected to exactly one vertex on the boundary of the environment ∂E. Then the degeneracy $deg = 2^{N_{\partial B}}$. A general proof of formula (1.59) is given in the next section § 1.3.2 . The subspace spanned by the degenerate ground states is called the *ground space*, with the dimension given by deg in (1.59). We emphasize at this point that the block B should contain more than one vertices, otherwise we have a trivial case that the block Hamiltonian vanishes $H_B = 0$ and the whole Hilbert space become the *ground space*. We discuss the density matrix for a single vertex block at the end of § 1.3.3 . The spectrum of the density

matrix $\boldsymbol{\rho}_B$ is closely related to the block Hamiltonian. The density matrix is a projector onto the ground space multiplied by another matrix. We shall prove this statement for an arbitrary graph or lattice in § 1.3.3 .

1.3.2 The Degeneracy of Ground States

We prove Katsura's formula (1.59) for the degeneracy of ground states of the block Hamiltonian. The proof applies to both the basic and the generalized models. The block Hamiltonian is defined in (1.58). Let us first look at the uniqueness condition (1.23). (The condition (1.15) for the basic model is a special case of this general one.) For an arbitrary vertex (site) l in the block B, the condition can be written as

$$2S_l = \sum_k M_{kl} = \sum_{k\in B} M_{kl} + \sum_{k\in\partial E} M_{kl}, \qquad l \in B. \tag{1.60}$$

Note that the sum over vertices $k \in \partial E$ is *outside* the block B. These terms are only present for boundary vertices $l \in \partial B$. Expression (1.60) is valid for *any* vertex in the block (for a bulk vertex the last summation vanishes). Next we define *the block VBS state*

$$|\mathrm{VBS}_{N_B}\rangle = \prod_{\langle kl\rangle\in B} \left(a_k^\dagger b_l^\dagger - b_k^\dagger a_l^\dagger\right)^{M_{kl}} |\mathrm{vac}\rangle, \qquad k \in B, \quad l \in B. \tag{1.61}$$

Here edge (bond) $\langle kl\rangle$ lies completely inside the block B. Now an *arbitrary* ground state of the block Hamiltonian H_B takes the following form

$$|\mathrm{G}\rangle = \left[\prod_{l\ \in\ \partial B}^{N_{\partial B}\ \text{terms}} f(a_l^\dagger, b_l^\dagger)\right] |\mathrm{VBS}_{N_B}\rangle, \tag{1.62}$$

where $f(a_l^\dagger, b_l^\dagger)$ is a polynomial (it may depend on the vertex l) in $a_l^\dagger$ and $b_l^\dagger$ and the product runs over all boundary vertices (with the total number denoted by $N_{\partial B}$). The degree of this polynomial is equal to $\sum_{k\in\partial E} M_{kl}$. (Each term in the polynomial must have the same total power $\sum_{k\in\partial E} M_{kl}$ of $a_l^\dagger$ and $b_l^\dagger$.) It is straightforward to verify that $|\mathrm{G}\rangle$ in (1.62) is a ground state:

1. The power of $a_l^\dagger$ and $b_l^\dagger$ in $|\mathrm{VBS}_{N_B}\rangle$ is $\sum_{k\in B} M_{kl}$ (see (1.61)), so that the total power of $a_l^\dagger$ and $b_l^\dagger$ in (1.62) is $\sum_{k\in B} M_{kl} + \sum_{k\in\partial E} M_{kl} = 2S_l$ according to (1.60). Therefore, we have the correct power $2S_l$ of the bosonic operators $a_l^\dagger$ and $b_l^\dagger$ for each vertex l in the block B (constraint (1.28) is satisfied);

2. There is no projection on any bond (edge) spin value greater than or equal to $S_k + S_l - M_{kl} + 1$ because of the construction of the block VBS state (1.61). (One could use the same reasoning as in § 1.2.4).

Therefore the degeneracy *deg* of the ground states of H_B is equal to the number of linearly independent states of the form (1.62). Since $a_l^\dagger$'s and $b_l^\dagger$'s are bosonic and commute, the number of linearly independent polynomials $f(a_l^\dagger, a_l^\dagger)$ for an arbitrary l is equal to its degree plus one, *i.e.* $\left(\sum_{k\in\partial E} M_{kl}\right) + 1$, $\forall\ l \in \partial B$. So that the total number of linearly independent polynomials of the form $\prod_{l\ \in\ \partial B}^{N_{\partial B}\ \text{terms}} f(a_l^\dagger, b_l^\dagger)$ is the product of these numbers for each $l \in \partial B$. Finally, the ground state degeneracy of the block Hamiltonian H_B is (Katsura's formula)

$$deg = \prod_{l\in\partial B} \left[\left(\sum_{k\in\partial E} M_{kl} \right) + 1 \right]. \tag{1.63}$$

In the case of the basic model all $M_{kl} = 1$, formula (1.63) has a graphical illustration, see Figure 1.2. We count the number # of all cut edges (dashed lines) incident to one boundary vertex of the block, then add one to the number #. The degeneracy is the product of these $(\# + 1)$'s for each boundary vertex.

1.3.3 General Properties of the Density Matrix

The reduced density matrix $\boldsymbol{\rho}_B$ from a VBS state has important and special spectrum structures which are universal among AKLT models. Let us denote by N_B the number of vertices in the block B. Then the dimension *dim* of the Hilbert space of the block B is equal to $\prod_l (2S_l + 1)$ with $l \in B$, which is also the dimension of the density matrix $\boldsymbol{\rho}_B$. The value is

$$dim = \prod_{l\in B} \left[z_l + 1 \right], \tag{1.64}$$

for the basic model and

$$dim = \prod_{l\in B} \left[\left(\sum_{k\in(B\cup\partial E)} M_{kl} \right) + 1 \right], \tag{1.65}$$

for the generalized model. In both expressions (1.64) and (1.65) we have N_B factors in the product. Take, for example, a particularly simple basic model in which each vertex is connected with the same number z of vertices, including those corresponding to boundary vertices (such as in the case of a lattice).

Then the dimension $dim = (z+1)^{N_B}$. The density matrix $\boldsymbol{\rho}_B$ would have dim number of eigenvalues. However, most of the eigenvalues are vanishing and $\boldsymbol{\rho}_B$ is a projector onto a much smaller subspace multiplied by another matrix. To prove this statement, we define a *support* to be the subspace of the Hilbert space of the block B with non-zero eigenvalues, *i.e.* it is spanned by eigenstates of $\boldsymbol{\rho}_B$ with non-zero eigenvalues. The dimension of the support is denoted by D. Then We have the following theorem on the structure of the density matrix $\boldsymbol{\rho}_B$ (Assuming that the block have more than one vertices, *i.e.* $N_B \geq 2$, so that H_B is not equal to zero identically):

Theorem 1.1

The *support* of $\boldsymbol{\rho}_B$ (1.54) is a subspace of the *ground space* of the block Hamiltonian H_B (1.58).

To prove the theorem, we recall that $H = \sum_{\langle kl\rangle \in B} H(k,l)$ and each $H(k,l)$ is a sum of projectors (1.22). We have $H(k,l) \geq 0$. Then the construction of the VBS ground state (1.20) and (1.31) guarantees that there is no projection onto the subspace with higher bond spins ($J \geq S_k + S_l - M_{kl} + 1$) for *any* bond (edge). (See § 1.2.5 for the proof.) Therefore,

$$H(k,l)|\mathrm{VBS}\rangle = 0, \qquad \forall\ \langle kl\rangle. \tag{1.66}$$

In particular, this is true for bonds (edges) *inside* the block B, *i.e.* both $k \in B$ and $l \in B$. Now, from the definition of $\boldsymbol{\rho}_B$ in (1.54), we have

$$\begin{aligned} H(k,l)\boldsymbol{\rho}_B &= H(k,l)\mathrm{tr}_E[\ \boldsymbol{\rho}\ ] \\ &= \frac{H(k,l)\mathrm{tr}_E[\ |\mathrm{VBS}\rangle\langle\mathrm{VBS}|\ ]}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle} \\ &= \frac{\mathrm{tr}_E[\ H(k,l)|\mathrm{VBS}\rangle\langle\mathrm{VBS}|\ ]}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle} \\ &= 0, \qquad k \in B, \quad l \in B. \end{aligned} \tag{1.67}$$

In the last step of (1.67) we have used (1.66) and the fact that bond (edge) $\langle kl\rangle$ lies completely inside the block B so that $H(k,l)$ commutes with the tracing operation in the environment E. Equation (1.67) is true for any bond (edge) in B, so that

$$H_B\boldsymbol{\rho}_B = \sum_{\langle kl\rangle \in B} H(k,l)\boldsymbol{\rho}_B = 0, \qquad k \in B, \quad l \in B. \tag{1.68}$$

If we diagonalize the density matrix $\boldsymbol{\rho}_B$

$$\boldsymbol{\rho}_B = \sum_{\lambda \neq 0} \lambda |\lambda\rangle\langle\lambda|, \tag{1.69}$$

where $|\lambda\rangle$ is the eigenstate corresponding to eigenvalue λ. Then (1.68) can be re-written as

$$H_B \sum_{\lambda \neq 0} \lambda |\lambda\rangle\langle\lambda| = \sum_{\lambda \neq 0} \lambda H_B |\lambda\rangle\langle\lambda| = 0, \tag{1.70}$$

Note that $\{|\lambda\rangle\}$ is a linearly independent set. Therefore the solution of (1.70) means that

$$H_B|\lambda\rangle = 0, \qquad \lambda \neq 0. \tag{1.71}$$

Expression (1.71) states that any eigenstate of $\boldsymbol{\rho}_B$ (with non-zero eigenvalue) is a ground state of H_B. As a result, we have proved **Theorem 1.1** that the *support* of $\boldsymbol{\rho}_B$ is a subspace of the *ground space* of H_B, so that $D \leq deg$. The density matrix takes the form of a projector multiplied by another matrix (a constant matrix depending on non-vanishing eigenvalues) and the projector projects on the *ground space*. Also, it is clear from expressions (1.59) and (1.64), (1.65) that $deg \leq dim$ ($\partial B \subseteq B$ so that $N_{\partial B} \leq N_B$). Usually, deg is much smaller than dim because the former involves only contributions from boundary vertices (sites) of the block while the latter also involves contributions from all bulk vertices (sites). Then as a corollary of **Theorem 1.1**, we have

$$D \leq deg \leq dim. \tag{1.72}$$

If the block B consists of only one vertex with a spin-S, then we *conjecture* that it is in the maximally entangled state. The *support* has dimension $D = 2S + 1$.

1.4 The 1–Dimensional Spin–1 Basic Model

One of the most simple models is defined on a 1-dimensional lattice with spin-1's in the bulk and spin-1/2's at both ends. We shall denote by $\boldsymbol{S}_j$ the vector

spin operator at site j ($j = 0, 1, \ldots, N+1$). The Hamiltonian is

$$H = \frac{1}{2}\sum_{j=1}^{N-1}\left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + \frac{1}{3}\left(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\right)^2 + \frac{2}{3}\right) + \pi_{\frac{3}{2}}(0,1) + \pi_{\frac{3}{2}}(N, N+1). \tag{1.73}$$

Each bulk term is a projector π_2 onto the states with bond spin-2. The boundary terms $\pi_{\frac{3}{2}}$ describe interactions of a spin-1/2 on the boundary and a spin-1 in the bulk. Each term is a projector onto the states with bond spin-3/2:

$$\pi_{\frac{3}{2}}(0,1) = \frac{2}{3}\left(1 + \boldsymbol{S}_0 \cdot \boldsymbol{S}_1\right), \qquad \pi_{\frac{3}{2}}(N, N+1) = \frac{2}{3}\left(1 + \boldsymbol{S}_N \cdot \boldsymbol{S}_{N+1}\right). \tag{1.74}$$

The choice of boundary terms guarantees the uniqueness of the ground state. As mentioned before, if we have spin-1 at every site in (1.73) instead, the ground state would become 4-fold degenerate.

1.4.1 The VBS Ground State

Given the Hamiltonian (1.73), we are going to use the graphical method (see § 1.2.3) to construct the unique VBS ground state. In order to represent the state, we first introduce the following notation for convenience [11]:

$$|\alpha\rangle \equiv (-1)^{1+\delta_{\alpha,0}} I \otimes \sigma_\alpha |0\rangle, \qquad \alpha = 0, 1, 2, 3 \tag{1.75}$$

where $\sigma_0 \equiv I$ (2-dimensional identity), $\sigma_{\alpha=1,2,3}$ are standard Pauli matrices and $|0\rangle \equiv \frac{-1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is the singlet state (antisymmetric projection) of two spin-1/2's. (It corresponds to the antisymmetrized state $|\Phi\rangle$ in § 1.2.3 .) These four states (1.75) (called *maximally entangled states*) form an orthonormal basis of the Hilbert space of two spin-1/2 operators.

The spin-1 state at each site is represented by a symmetric projection of two spin-1/2 states given by (1.75) for $\alpha = 1, 2, 3$. Let us take the j^{th} site for example, see Figure 1.3. The two spin-1/2's are labeled by $(j, \bar{j})$ (from left to right, respectively). Then the spin-1 states are prepared by projecting these two spin-1/2's (4-dimensional space) onto a symmetric 3-dimensional subspace

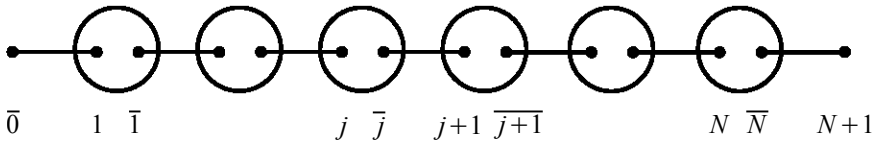

Figure 1.3: Graphical representation of the VSB ground state for the 1-dimensional spin-1 model: Each spin-1 is realized by a pair of spin-$\frac{1}{2}$'s which are represented by small black dots in the figure. The pair of spin-$\frac{1}{2}$ states at site j are labeled j, $\bar{j}$. The solid lines connecting two neighboring dots ($\bar{j}$ and $j+1$) represent anti-symmetrization of two spin-$\frac{1}{2}$'s; The large circles enclosing two dots (j and $\bar{j}$) represent symmetrization at each site. The boundary spin-$\frac{1}{2}$'s are labeled $\bar{0}$ and $N+1$ in consistency with the prescription.

spanned by

$$\begin{aligned} |1\rangle_{j\bar{j}} &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_j|\uparrow\rangle_{\bar{j}} - |\downarrow\rangle_j|\downarrow\rangle_{\bar{j}}), \\ |2\rangle_{j\bar{j}} &= \frac{-i}{\sqrt{2}}(|\uparrow\rangle_j|\uparrow\rangle_{\bar{j}} + |\downarrow\rangle_j|\downarrow\rangle_{\bar{j}}), \\ |3\rangle_{j\bar{j}} &= \frac{-1}{\sqrt{2}}(|\uparrow\rangle_j|\downarrow\rangle_{\bar{j}} + |\downarrow\rangle_j|\uparrow\rangle_{\bar{j}}). \end{aligned} \tag{1.76}$$

Thus the two ending spin-1/2's are labeled as site $\bar{0}$ and $N+1$, consistently (Figure 1.3). The unique VBS ground state in this representation is [1, 2, 11]

$$|\mathrm{VBS}\rangle = \left(\bigotimes_{j=1}^{N} \mathbf{P}_{j\bar{j}}\right) |0\rangle_{\bar{0}1}|0\rangle_{\bar{1}2}\cdots|0\rangle_{\bar{N}N+1}. \tag{1.77}$$

Here $\mathbf{P}_{j\bar{j}}$ projects two spin-1/2 states onto a symmetric subspace, which describes spin-1. Using basis (1.75), we have

$$\mathbf{P}_{j\bar{j}} = \sum_{\alpha=1}^{3} |\alpha\rangle_{j\bar{j}}\langle\alpha|. \tag{1.78}$$

This projector $\mathbf{P}_{j\bar{j}}$ serves the same purpose as the symmetrization operator $\mathbf{P}(l)$ in § 1.2.3 and their results acting on a product state of spin-$\frac{1}{2}$'s only differ by a normalization. We use the projector $\mathbf{P}_{j\bar{j}}$ for convenience here.

A crucial step (see [11]) is that the ground state (1.77) can be expressed in

a different form using the following identity

$$|0\rangle_{\bar{A}B}|0\rangle_{\bar{B}C} = \frac{-1}{2}\sum_{\alpha=0}^{3}|\alpha\rangle_{B\bar{B}}\left[I_{\bar{A}}\otimes(\sigma_\alpha)_C\right]|0\rangle_{\bar{A}C} \tag{1.79}$$

for arbitrary labels (indices) A, B and C. This identity (1.79) can be verified by direct calculation and comparison. Repeatedly using relation (1.79), the product of $|0\rangle$'s in (1.77) can be re-written as

$$\begin{aligned} & |0\rangle_{\bar{0}1}|0\rangle_{\bar{1}2}\cdots|0\rangle_{\bar{N}N+1} \\ = & \left(\frac{-1}{2}\right)^N \sum_{\alpha_1,\cdots,\alpha_N=0}^{3}|\alpha_1\rangle\cdots|\alpha_N\rangle\left[I_{\bar{0}}\otimes(\sigma_{\alpha_N}\cdots\sigma_{\alpha_1})_{N+1}\right]|0\rangle_{\bar{0}N+1}. \end{aligned} \tag{1.80}$$

Then by projecting onto the symmetric subspace spanned by $|\alpha = 1, 2, 3\rangle$, the ground VBS state (1.77) takes the form [15, 49]

$$|\mathrm{VBS}\rangle = \frac{1}{3^{N/2}}\sum_{\alpha_1,\cdots,\alpha_N=1}^{3}|\alpha_1\rangle\cdots|\alpha_N\rangle\left[I_{\bar{0}}\otimes(\sigma_{\alpha_N}\cdots\sigma_{\alpha_1})_{N+1}\right]|0\rangle_{\bar{0}N+1}. \tag{1.81}$$

Note that this ground state (1.81) is normalized and we have re-written the overall phase for it has no physical content.

1.4.2 The Block Density Matrix

Given the ground state in the form (1.81), we obtain the density matrix of a block of L contiguous bulk spins starting at site k by tracing out spin degrees of freedom outside the block using basis (1.75):

$$\boldsymbol{\rho}_L \equiv \mathrm{tr}_{\bar{0},1,\ldots,k-1,k+L,\ldots,N,N+1}\left[\,|\mathrm{VBS}\rangle\langle\mathrm{VBS}|\,\right]. \tag{1.82}$$

(Note that we use subscript L to emphasize the dependence of the density matrix on the size of the block instead of using the general B as representing 'block'.) In taking the partial trace, we will encounter the following expression in calculation

$$I_n = \sum_{\sigma_{\alpha_1},\cdots,\sigma_{\alpha_n}=1}^{3} I\otimes(\sigma_{\alpha_n}\cdots\sigma_{\alpha_1})\,|0\rangle\langle 0|\;I\otimes(\sigma_{\alpha_1}\cdots\sigma_{\alpha_n})\,, \qquad n\geq 1 \tag{1.83}$$

given $I_0 = |0\rangle\langle 0|$. To solve this (1.83), we introduce iterative coefficients A_n and B_n and write

$$I_n = A_n|0\rangle\langle 0| + B_n \sum_{\beta=1}^{3} |\beta\rangle\langle\beta|, \qquad n \geq 1. \tag{1.84}$$

Then from (1.83) we could write down the expression of I_{n+1} in terms of A_n and B_n. Comparison of coefficients yields the following iteration relation

$$A_{n+1} = 3B_n, \qquad B_{n+1} = A_n + 2B_n, \qquad n \geq 1 \tag{1.85}$$

with $A_0 = 1$ and $B_0 = 0$. The solution to (1.85) is

$$A_n = \frac{1}{4}\left(3^n + 3(-1)^n\right), \qquad B_n = \frac{1}{4}\left(3^n - (-1)^n\right). \tag{1.86}$$

As a result, we have found that

$$I_n = \frac{1}{4}\left(3^n + 3(-1)^n\right)|0\rangle\langle 0| + \frac{1}{4}\left(3^n - (-1)^n\right)\sum_{\beta=1}^{3} |\beta\rangle\langle\beta|. \tag{1.87}$$

Using (1.87), it is straightforward to take the partial trace in (1.82). The result is independent of the starting site k and the total length N (see [11]). (So that the density matrix is translational invariant though the whole spin chain Hamiltonian does not have complete translational invariance because of the boundary conditions.) We choose $k = 1$ (*i.e.* re-label the indices of sites for notational convenience) so that the density matrix reads [11]

$$\boldsymbol{\rho}_L = \frac{1}{3^L}\sum_{\alpha,\alpha'=1}^{3} |\alpha_1\rangle\langle\alpha_1'|\cdots|\alpha_L\rangle\langle\alpha_L'|\langle 0|I\otimes(\sigma_{\alpha_1'}\cdots\sigma_{\alpha_L'})I\otimes(\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})|0\rangle. \tag{1.88}$$

1.4.3 Ground States of the Block Hamiltonian

The block in 1-dimension is L contiguous bulk spins. The block Hamiltonian H_B by definition (1.58) reads

$$H_B = \frac{1}{2}\sum_{j=1}^{L-1}\left(\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1} + \frac{1}{3}\left(\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1}\right)^2 + \frac{2}{3}\right). \tag{1.89}$$

Any linear combination of states of the following form

$$|\mathrm{G};\chi_1,\chi_{\bar{L}}\rangle \equiv \left(\bigotimes_{j=1}^{L}\mathbf{P}_{j\bar{j}}\right)|\chi_1\rangle_1|0\rangle_{\bar{1}2}|0\rangle_{\bar{2}3}\cdots|0\rangle_{\overline{L-1}L}|\chi_{\bar{L}}\rangle_{\bar{L}} \tag{1.90}$$

is a ground state of the block Hamiltonian (1.89). In (1.90) we have made notation $|\chi\rangle \equiv |\uparrow \text{ or } \downarrow\rangle$ represents the two spin-1/2 states and $\mathbf{P}_{j\bar{j}}$ is defined in (1.78). Let us make a particular linear combination of these $|\mathrm{G};\chi_1,\chi_{\bar{L}}\rangle$ states using (1.75) and write the four ($\alpha = 0,1,2,3$) linearly independent ground states of the block Hamiltonian (1.89) as follows

$$|\mathrm{VBS};\alpha\rangle \equiv \left(\bigotimes_{j=1}^{L}\mathbf{P}_{j\bar{j}}\right)|\alpha\rangle_{\bar{L}1}|0\rangle_{\bar{1}2}|0\rangle_{\bar{2}3}\cdots|0\rangle_{\overline{L-1}L}. \tag{1.91}$$

Note that we have changed the label G to VBS and these 4 states in (1.91) are called *degenerate VBS states*. Now we go through the same steps as from (1.77) to (1.81), the resultant form of the four ground states ($\alpha = 0,1,2,3$) is

$$|\mathrm{VBS};\alpha\rangle = \sum_{\alpha_1,\cdots,\alpha_L=1}^{3}|\alpha_1\rangle\cdots|\alpha_L\rangle\ \langle\alpha_L|\sigma_\alpha\otimes\left(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1}\right)|0\rangle. \tag{1.92}$$

Again we have re-written the overall phase for simplicity. These four states are orthogonal, and the normalization is given by (the calculation is similar to that of A_n and B_n in (1.85))

$$\langle\mathrm{VBS};\alpha|\mathrm{VBS};\alpha\rangle = \begin{cases} \frac{1}{4}(3^L+3(-1)^L), & \alpha = 0; \\ \\ \frac{1}{4}(3^L-(-1)^L), & \alpha = 1,2,3. \end{cases} \tag{1.93}$$

1.4.4 Spectrum of the Density Matrix

According to **Theorem 1.1**, the eigenvectors corresponding to non-zero eigenvalues of the density matrix (1.88) are degenerate ground states of the block Hamiltonian (1.89). These are exactly the degenerate VBS states found in (1.92). Let us apply $\boldsymbol{\rho}_L$ to $|\mathrm{VBS};\alpha\rangle$ and use orthogonality of the $|\alpha\rangle$ states. Then we obtain

$$\boldsymbol{\rho}_L|\mathrm{VBS};\alpha\rangle = \frac{1}{3^L}\sum_{\alpha_1,\cdots,\alpha_L=1}^{3}|\alpha_1\rangle\cdots|\alpha_L\rangle\ C_{\alpha_1\cdots\alpha_L} \tag{1.94}$$

with coefficient

$$C_{\alpha_1\cdots\alpha_L} = \sum_{\alpha'_1,\cdots,\alpha'_L=1}^{3} \langle\alpha'_L|\sigma_\alpha\otimes(\sigma_{\alpha'_{L-1}}\cdots\sigma_{\alpha'_1})|0\rangle \cdot\langle 0|I\otimes(\sigma_{\alpha'_1}\cdots\sigma_{\alpha'_L})I\otimes(\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})|0\rangle. \tag{1.95}$$

Using the same method of induction as in obtaining A_n and B_n in (1.85), we have

$$\sum_{\alpha'_1,\cdots,\alpha'_{L-1}=1}^{3}(I\otimes\sigma_{\alpha'_{L-1}}\cdots\sigma_{\alpha'_1})|0\rangle\langle 0|(I\otimes\sigma_{\alpha'_1}\cdots\sigma_{\alpha'_{L-1}}) = \sum_{\beta=0}^{3}A_\beta|\beta\rangle\langle\beta| \tag{1.96}$$

with

$$A_\beta = \begin{cases} \frac{1}{4}(3^{L-1}+3(-1)^{L-1}), & \beta=0; \\ \\ \frac{1}{4}(3^{L-1}-(-1)^{L-1}), & \beta=1,2,3. \end{cases} \tag{1.97}$$

Therefore the coefficient $C_{\alpha_1\cdots\alpha_L}$ defined in (1.95) can be simplified as

$$C_{\alpha_1\cdots\alpha_L} = \sum_{\alpha'_L=1,\beta=0}^{3} A_\beta\langle\alpha'_L|\sigma_\alpha\otimes I|\beta\rangle\langle\beta|I\otimes(\sigma_{\alpha'_L}\sigma_{\alpha_L})I\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle. \tag{1.98}$$

Straightforward calculation using multiplication rules of Pauli matrices shows that (1.98) can be further simplified as

$$\begin{aligned} C_{\alpha_1\cdots\alpha_L} &= 3A_1\delta_{\alpha,0}\langle\alpha_L|I\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle \\ &+(A_0+2A_1)(1-\delta_{\alpha,0})(\delta_{\alpha\alpha_L}\langle 0|-\mathrm{i}\sum_{\beta=1}^{3}\epsilon_{\alpha\alpha_L\beta}\langle\beta|)I\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle \end{aligned} \tag{1.99}$$

where $\epsilon_{\alpha\alpha_L\beta}$ is the totally antisymmetric tensor of three indices with $\epsilon_{123}=1$. By realizing that

$$\delta_{\alpha\alpha_L}\langle 0|-\mathrm{i}\sum_{\beta=1}^{3}\epsilon_{\alpha\alpha_L\beta}\langle\beta| = \langle 0|\sigma_{\alpha_L}\sigma_\alpha\otimes I = \langle\alpha_L|\sigma_\alpha\otimes I, \tag{1.100}$$

we have reached the final form of the coefficient $C_{\alpha_1\cdots\alpha_L}$ such that

$$C_{\alpha_1\cdots\alpha_L} = [3A_1\delta_{\alpha,0} + (A_0+2A_1)(1-\delta_{\alpha,0})]\,\langle\alpha_L|\sigma_\alpha\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle. \tag{1.101}$$

As a result, we plug (1.101) into (1.94) and find that

$$\begin{aligned}\boldsymbol{\rho}_L|\mathrm{VBS};\alpha\rangle &= \frac{3A_1\delta_{\alpha,0}+(A_0+2A_1)(1-\delta_{\alpha,0})}{3^L} \\ &\cdot\sum_{\alpha_1,\cdots,\alpha_L=1}^{3}|\alpha_1\rangle\cdots|\alpha_L\rangle\langle\alpha_L|\sigma_\alpha\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle.\end{aligned} \tag{1.102}$$

By comparing with (1.92), we find that (1.102) is exactly the statement that $|\mathrm{VBS};\alpha\rangle$ ($\alpha=0,1,2,3$) are eigenvectors of the density matrix $\boldsymbol{\rho}_L$:

$$\boldsymbol{\rho}_L|\mathrm{VBS};\alpha\rangle = \Lambda_\alpha|\mathrm{VBS};\alpha\rangle, \qquad \alpha=0,1,2,3 \tag{1.103}$$

with eigenvalues

$$\Lambda_\alpha = \frac{3A_1\delta_{\alpha,0}+(A_0+2A_1)(1-\delta_{\alpha,0})}{3^L} = \begin{cases} \frac{1}{4}(1+3(-\frac{1}{3})^L), & \alpha=0; \\ \\ \frac{1}{4}(1-(-\frac{1}{3})^L), & \alpha=1,2,3. \end{cases} \tag{1.104}$$

These numbers obtained in (1.104) are exactly the eigenvalues found in [11, 32] for spin-1, and are consistent with our later explicit expression for eigenvalues in the more general case, see (1.186) in § 1.5.6 .

We can also prove explicitly that any other eigenvectors of $\boldsymbol{\rho}_L$ orthogonal to the set $\{|\mathrm{VBS};\alpha\rangle\}$ have zero eigenvalue. Note that a complete basis of the Hilbert space $\mathbf{H}_L$ of the block of spins can be chosen as

$$\{|\alpha_1\rangle\cdots|\alpha_L\rangle\}, \qquad \alpha=1,2,3. \tag{1.105}$$

The subspace $\mathbf{H}_\Lambda$ with non-zero eigenvalues is panned by $\{|\mathrm{VBS};\alpha\rangle\}$, as we have already shown. The Hilbert space can be reduced into a direct sum

$$\mathbf{H}_L = \mathbf{H}_\Lambda\oplus\mathbf{H}_\Phi. \tag{1.106}$$

We will show that the subspace $\mathbf{H}_\Phi$ orthogonal to $\mathbf{H}_\Lambda$ is a subspace of vanishing eigenvalues. Mathematically, this means that for an arbitrary basis vector

$|\beta_1\rangle\cdots|\beta_L\rangle$, we shall have

$$\boldsymbol{\rho}_L(\mathbf{I}_L-\mathbf{P}_\Lambda)|\beta_1\rangle\cdots|\beta_L\rangle=0, \tag{1.107}$$

where $\mathbf{I}_L$ is the identity of $\mathbf{H}_L$ and $\mathbf{P}_\Lambda$ is the projector onto $\mathbf{H}_\Lambda$:

$$\begin{aligned}\mathbf{I}_L &\equiv \sum_{\alpha_1,\cdots,\alpha_L=1}^{3}|\alpha_1\rangle\cdots|\alpha_L\rangle\langle\alpha_1|\cdots\langle\alpha_L|,\\ \mathbf{P}_\Lambda &\equiv \sum_{\alpha=1}^{3}\frac{|\mathrm{VBS};\alpha\rangle\langle\mathrm{VBS};\alpha|}{\langle\mathrm{VBS};\alpha|\mathrm{VBS};\alpha\rangle}.\end{aligned} \tag{1.108}$$

By taking expressions (1.88), (1.108), (1.103), and realizing that

$$\sum_{\alpha=0}^{3}\frac{3^L\Lambda_\alpha}{\langle\mathrm{VBS};\alpha|\mathrm{VBS};\alpha\rangle}|\alpha\rangle\langle\alpha|=\sum_{\alpha=0}^{3}|\alpha\rangle\langle\alpha|=I\otimes I, \tag{1.109}$$

we find the left hand side of (1.107) being equal to

$$\begin{aligned}&\boldsymbol{\rho}_L(\mathbf{I}_L-\mathbf{P}_\Lambda)|\beta_1\rangle\cdots|\beta_L\rangle \\ =\ &\frac{1}{3^L}\sum_{\alpha_1\cdots\alpha_L=1}^{3}|\alpha_1\rangle\cdots|\alpha_L\rangle\ \langle 0|[I\otimes(\sigma_{\beta_1}\cdots\sigma_{\beta_L}),I\otimes(\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})]|0\rangle.\end{aligned} \tag{1.110}$$

We use multiplication rules of Pauli matrices to write the two terms within the commutator in (1.110) as

$$\begin{aligned}I\otimes(\sigma_{\beta_1}\cdots\sigma_{\beta_L})&=\mathrm{e}^{\mathrm{i}\theta(\beta)}I\otimes\sigma_\beta, \qquad \beta=0,1,2,3;\\ I\otimes(\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})&=\mathrm{e}^{\mathrm{i}\theta(\alpha)}I\otimes\sigma_\alpha, \qquad \alpha=0,1,2,3.\end{aligned} \tag{1.111}$$

Here $\mathrm{e}^{\mathrm{i}\theta(\beta)}$ and $\mathrm{e}^{\mathrm{i}\theta(\alpha)}$ are two phase factors. Then the commutator is

$$[I\otimes(\sigma_{\beta_1}\cdots\sigma_{\beta_L}),I\otimes(\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})]=\mathrm{e}^{\mathrm{i}(\theta(\beta)+\theta(\alpha))}I\otimes[\sigma_\beta,\sigma_\alpha]. \tag{1.112}$$

There are two possibilities:

1. $\alpha=\beta$ or at least one of the two is equal to zero, then σ_β and σ_α commutes;
2. $\alpha\neq\beta\neq 0$, then $[\sigma_\beta,\sigma_\alpha]=2\mathrm{i}\sum_{\gamma=1}^{3}\epsilon_{\beta\alpha\gamma}\sigma_\gamma$, but we still have $\langle 0|I\otimes\sigma_\gamma|0\rangle=\langle 0|\gamma\rangle=0$.

Therefore, the factor $\langle 0|[I\otimes(\sigma_{\beta_1}\cdots\sigma_{\beta_L}),I\otimes(\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})]|0\rangle$ in (1.110) is identically zero. So that we have proved (1.107). Therefore $\mathbf{H}_\Phi$ is a subspace with

only zero eigenvalues.

1.4.5 The Large Block Limit

It is interesting to study the large block limit that $L \to \infty$. We recognized from (1.104) that all four eigenvalues approach the same limit

$$\Lambda_\alpha = \frac{1}{4}, \qquad L \to \infty. \tag{1.113}$$

As a result, the von Neumann entropy coincides with the Rényi entropy in the numerical value and both equal to

$$S_{\text{v N}} = S_{\text{R}}(\alpha) = 2\ln 2, \qquad L \to \infty. \tag{1.114}$$

The limiting density matrix $\boldsymbol{\rho}_L$ is proportional to the projector $\mathbf{P}_\Lambda$ (1.108) which projects on the 4-degenerate ground states (the ground space) of the block Hamiltonian, *i.e.*

$$\boldsymbol{\rho}_L = \frac{1}{4}\mathbf{P}_\Lambda, \qquad L \to \infty. \tag{1.115}$$

1.5 The 1-dimensional Spin-S Homogeneous Model

In 1-dimension, if all bulk spins take the same value S, the model is called the *homogeneous* model. The system consists of a linear chain of N spin-S's in the bulk, and two spin-$\frac{1}{2}S$'s on the boundaries. Let $\boldsymbol{S}_j$ denotes the vector spin operator at site j ($j = 0, 1, \ldots, N+1$). The Hamiltonian is

$$H = \sum_{j=1}^{N-1} \sum_{J=S+1}^{2S} C_J(j, j+1)\pi_J(j, j+1) + H(0,1) + H(N, N+1), \tag{1.116}$$

where the projector $\pi_J(j, j+1)$ projects the bond spin $\boldsymbol{J}_{j,j+1} \equiv \boldsymbol{S}_j + \boldsymbol{S}_{j+1}$ onto the subspace with total spin J ($J = S+1, \ldots, 2S$). Physically formation of bond spins with these values would increase energy. The boundary terms

describe interactions between a spin-$S/2$ and a spin-S:

$$\begin{aligned} H(0,1) &= \sum_{J=S/2+1}^{3S/2} C_J(0,1)\pi_J(0,1), \\ H(N,N+1) &= \sum_{J=S/2+1}^{3S/2} C_J(N,N+1)\pi_J(N,N+1). \end{aligned} \tag{1.117}$$

Coefficients $C_J(j,j+1)$ can take arbitrary positive values. This model is a special case of the generalized model in 1-dimension with all multiplicity number $M_{j,j+1} = S$.

1.5.1 The VBS ground State

The Construction of VBS State

According to the general approach in § 1.2.4 , the unique VBS ground state of the Hamiltonian (1.116) is constructed in the Schwinger representation as [4]

$$|\text{VBS}\rangle \equiv \prod_{j=0}^{N} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger \right)^S |\text{vac}\rangle, \tag{1.118}$$

where $a^\dagger$, $b^\dagger$ are bosonic creation operators and $|\text{vac}\rangle$ is destroyed by any of the annihilation operators a, b. Recall that these operators satisfy $[a_i, a_j^\dagger] = [b_i, b_j^\dagger] = \delta_{ij}$ with all other commutators vanishing. The spin operators are represented as $S_j^+ = a_j^\dagger b_j$, $S_j^- = b_j^\dagger a_j$, $S_j^z = (a_j^\dagger a_j - b_j^\dagger b_j)/2$. To reproduce the dimension of the spin-S Hilbert space at each site, an additional constraint on the total boson occupation number is required, namely $(a_j^\dagger a_j + b_j^\dagger b_j)/2 = S$. More details and properties of the VBS state in the Schwinger representation can be found in § 1.2.4 and [4, 5, 36]. The pure state density matrix of the VBS ground state (1.118) is

$$\boldsymbol{\rho} = \frac{|\text{VBS}\rangle\langle\text{VBS}|}{\langle\text{VBS}|\text{VBS}\rangle}. \tag{1.119}$$

We will discuss the normalization $\langle\text{VBS}|\text{VBS}\rangle$ of the VBS state after introducing the coherent state basis.

The Coherent State Basis

In order to calculate the normalization of the VBS state (1.118) and later the density matrix of the block, it is convenient to introduce a spin coherent state basis. We first introduce spinor coordinates

$$(u, v) \equiv \left(\cos\frac{\theta}{2} \mathrm{e}^{\mathrm{i}\frac{\phi}{2}}, \sin\frac{\theta}{2} \mathrm{e}^{-\mathrm{i}\frac{\phi}{2}} \right), \qquad 0 \leq \theta \leq \pi, \quad 0 \leq \phi \leq 2\pi. \tag{1.120}$$

Then for a point $\hat{\Omega} \equiv (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ on the unit sphere, the spin-S coherent state is defined as

$$|\hat{\Omega}\rangle \equiv \frac{\left(ua^\dagger + vb^\dagger\right)^{2S}}{\sqrt{(2S)!}}|\mathrm{vac}\rangle. \tag{1.121}$$

Here we have fixed the overall phase (a $U(1)$ gauge degree of freedom) since it has no physical content. Note that (1.121) is covariant under $SU(2)$ transforms (see § 1.5.8). The set of coherent states is complete (but not orthogonal) such that [18]

$$\frac{2S+1}{4\pi}\int \mathrm{d}\hat{\Omega}|\hat{\Omega}\rangle\langle\hat{\Omega}| = \sum_{m=-S}^{S} |S,m\rangle\langle S,m| = I_{2S+1}, \tag{1.122}$$

where $|S,m\rangle$ denote the eigenstate of $\boldsymbol{S}^2$ and S_z, and I_{2S+1} is the identity of the $(2S+1)$-dimensional Hilbert space for spin-S. To prove (1.122), we expand the expression (1.121) (see also (1.29))

$$|\hat{\Omega}\rangle = \sum_{m=-S}^{S} \sqrt{\frac{(2S)!}{(S+m)!(S-m)!}}\, u^{S+m} v^{S-m} |S,m\rangle. \tag{1.123}$$

Then, by substituting (1.123) into (1.122) and realizing that

$$\int \mathrm{d}\hat{\Omega}\; u^{S+m} v^{S-m} u^{*S+m'} v^{*S-m'} = \frac{(S+m)!(S-m)!}{(2S+1)!} 4\pi\delta_{mm'}, \tag{1.124}$$

the completeness relation (1.122) is then established. This relation (1.122) can be used in taking trace of an arbitrary operator.

Normalization of the VBS State

The VBS state $|\text{VBS}\rangle$ defined in (1.118) is not normalized. Using the coherent state formalism (1.121) and the completeness relation (1.122), we express the norm square as

$$\begin{aligned} & \langle \text{VBS}|\text{VBS}\rangle \qquad (1.125) \\ = & \left[\frac{(S+1)!}{4\pi}\right]^2 \left[\frac{(2S+1)!}{4\pi}\right]^N \int \left(\prod_{j=0}^{N+1} \mathrm{d}\hat{\Omega}_j\right) \prod_{j=0}^{N} \left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S \end{aligned}$$

where we have used

$$\langle 0|a^{S+l}b^{S-l}|\hat{\Omega}\rangle = \sqrt{(2S)!}\; u^{S+l}v^{S-l}. \qquad (1.126)$$

In order to carry out the integral in (1.125), we consider the expansion of the function $\left[\frac{1}{2}(1-x)\right]^S$ in terms of Legendre polynomials $P_l(x) = \frac{1}{2^l l!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^l (x^2-1)^l$ as follows

$$\left[\frac{1}{2}(1-x)\right]^S = \sum_{l=0}^{S} C_l P_l(x). \qquad (1.127)$$

The coefficient C_l is derived by using the orthogonality of P_l and repeatedly integrating by parts

$$\begin{aligned} C_l &= \frac{2l+1}{2}\int_{-1}^{1} \mathrm{d}x P_l(x)\left[\frac{1}{2}(1-x)\right]^S \\ &= \frac{2l+1}{2}\int_{-1}^{1} \mathrm{d}x \frac{1}{2^l l!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^l (x^2-1)^l \left[\frac{1}{2}(1-x)\right]^S \\ &= \frac{(2l+1)S!}{2^{S+l+1}l!(S-l)!}\int_{-1}^{1}\mathrm{d}x(x^2-1)^l(1-x)^{S-l} \\ &= \frac{(-1)^l(2l+1)S!}{2^{S+l+1}l!(S-l)!}\int_{-1}^{1}\mathrm{d}x(1-x)^S(1+x)^l \\ &= \frac{(-1)^l(2l+1)S!S!}{(S-l)!(S+l+1)!}. \qquad (1.128) \end{aligned}$$

Having expansion coefficients (1.128) and by replacing x with $\hat{\Omega}_j\cdot\hat{\Omega}_{j+1}$, the factor $\left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S$ under the integral of (1.125) can be expanded in terms of Legendre polynomials and further in terms of spherical harmonics by

further using

$$P_l(\hat{\Omega}_j \cdot \hat{\Omega}_{j+1}) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\hat{\Omega}_j) Y^*_{lm}(\hat{\Omega}_{j+1}). \tag{1.129}$$

The final result is [18, 32]

$$\begin{aligned} & \left[\frac{1}{2}(1 - \hat{\Omega}_j \cdot \hat{\Omega}_{j+1})\right]^S \\ = & \frac{1}{S+1} \sum_{l=0}^{S} (2l+1) \lambda(l,S) P_l(\hat{\Omega}_j \cdot \hat{\Omega}_{j+1}) \\ = & \frac{4\pi}{S+1} \sum_{l=0}^{S} \lambda(l,S) \sum_{m=-l}^{l} Y_{lm}(\hat{\Omega}_j) Y^*_{lm}(\hat{\Omega}_{j+1}) \end{aligned} \tag{1.130}$$

with coefficients $\lambda(l,S)$ given by

$$\lambda(l,S) \equiv \frac{(-1)^l S!(S+1)!}{(S-l)!(S+l+1)!}. \tag{1.131}$$

Now we expand $\left[\frac{1}{2}(1 - \hat{\Omega}_j \cdot \hat{\Omega}_{j+1})\right]^S$ in terms of spherical harmonics as in (1.130), then integrate from $\hat{\Omega}_0$ to $\hat{\Omega}_{N+1}$. We notice by using the orthogonality of spherical harmonics that each integral contributes a factor of $\frac{4\pi}{S+1}$ except the last one. For example,

$$\begin{aligned} & \int \mathrm{d}\hat{\Omega}_0 \left[\frac{1}{2}(1 - \hat{\Omega}_0 \cdot \hat{\Omega}_1)\right]^S \\ = & \frac{4\pi}{S+1} \sum_{l=0}^{S} \lambda(l,S) \sum_{m=-l}^{l} \sqrt{4\pi}\, Y^*_{lm}(\hat{\Omega}_1) \int \mathrm{d}\hat{\Omega}_0 Y_{lm}(\hat{\Omega}_0) Y^*_{00}(\hat{\Omega}_0) \\ = & \frac{4\pi}{S+1} \sqrt{4\pi}\, Y^*_{00}(\hat{\Omega}_1) = \frac{4\pi}{S+1}. \end{aligned} \tag{1.132}$$

The last integral over $\hat{\Omega}_{N+1}$ contributes simply a factor of 4π. Consequently, the norm square (1.125) is equal to

$$\langle \mathrm{VBS} | \mathrm{VBS} \rangle = \left[\frac{(2S+1)!}{S+1}\right]^N S!(S+1)!. \tag{1.133}$$

1.5.2 The Block Density Matrix

We take a block of L contiguous bulk spins as a subsystem. Now we calculate the block density matrix in the VBS state (1.118). By definition, this is achieved by taking the pure state density matrix (1.119) and tracing out all spin degrees of freedom outside the block:

$$\boldsymbol{\rho}_L \equiv \mathrm{tr}_{0,1,\ldots,k-1,k+L,\ldots,N,N+1} \left[\boldsymbol{\rho} \right], \qquad 1 \leq k, \quad k+L-1 \leq N. \tag{1.134}$$

Here the block of length L starts from site k and ends at site $k+L-1$. $\boldsymbol{\rho}_L$ is no longer a pure state density matrix because of entanglement of the block with the environment (sites outside the block of the spin chain). It was shown in [31, 50] that entries of the density matrix are multi-point correlation functions in the ground state. We give the proof of this statement for our spin-S case in § 1.5.9 .

Using the coherent state basis (1.121) and completeness relation (1.122), $\boldsymbol{\rho}_L$ can be written as [32]

$$\boldsymbol{\rho}_L = \tag{1.135}$$
$$\frac{\displaystyle\int \left[\prod_{j=0}^{k-1}\prod_{j=k+L}^{N+1} \mathrm{d}\hat{\Omega}_j\right] \prod_{j=0}^{k-2}\prod_{j=k+L}^{N} \left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S B^\dagger |\mathrm{VBS}_L\rangle\langle \mathrm{VBS}_L| B}{\displaystyle\left[\frac{(2S+1)!}{4\pi}\right]^L \int \left[\prod_{j=0}^{N+1} \mathrm{d}\hat{\Omega}_j\right] \prod_{j=0}^{N} \left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S}.$$

Here the boundary operator B and block VBS state $|\mathrm{VBS}_L\rangle$ are defined as

$$B \equiv (u_{k-1}b_k - v_{k-1}a_k)^S \, (a_{k+L-1}v_{k+L} - b_{k+L-1}u_{k+L})^S, \tag{1.136}$$

$$|\mathrm{VBS}_L\rangle \equiv \prod_{j=k}^{k+L-2} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\mathrm{vac}\rangle, \tag{1.137}$$

respectively. Note that both B and $|\mathrm{VBS}_L\rangle$ are $SU(2)$ covariant (see § 1.5.8). The expression (1.135) can be simplified. We can perform the integrals over $\hat{\Omega}_j$ ($j = 0, 1, \ldots, k-2, k+L+1, \ldots, N, N+1$) in the numerator and all integrals in the denominator (see § 1.5.1). After integrating over these variables, the density matrix $\boldsymbol{\rho}_L$ turns out to be independent of both the starting site k and the total length N of the spin chain. This property has been proved in [11] for spin $S = 1$ (using a different representation, namely the maximally entangled states, see § 1.4.2) and generalized in [32] for generic spin-S. Therefore, we can choose $k = 1$ (a relabeling for convenience) and the density matrix takes

the form

$$\boldsymbol{\rho}_L = \left[\frac{S+1}{(2S+1)!}\right]^L \frac{(S+1)}{(4\pi)^2} \int \mathrm{d}\hat{\Omega}_0 \mathrm{d}\hat{\Omega}_{L+1} B^\dagger |\mathrm{VBS}_L\rangle\langle \mathrm{VBS}_L| B \tag{1.138}$$

with

$$B^\dagger = \left(u_0^* b_1^\dagger - v_0^* a_1^\dagger\right)^S \left(a_L^\dagger v_{L+1}^* - b_L^\dagger u_{L+1}^*\right)^S, \tag{1.139}$$

$$|\mathrm{VBS}_L\rangle = \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\mathrm{vac}\rangle. \tag{1.140}$$

The state $|\mathrm{VBS}_L\rangle$ is called the block VBS state. The last two integral of (1.138) can be performed, but we keep its present form for later use.

1.5.3 Ground States of the Block Hamiltonian

Degenerate Ground States

In order to describe the eigenvectors and spectrum of the density matrix (1.138), we first study the zero-energy ground states of the block Hamiltonian. The block Hamiltonian is a collection of interacting terms within the block, *i.e.*

$$H_B = \sum_{j=1}^{L-1} \sum_{J=S+1}^{2S} C_J \pi_J(j, j+1). \tag{1.141}$$

Now we define a set of $S+1$ operators covariant under $SU(2)$ (see § 1.5.8)

$$A_J^\dagger \equiv \left(u a_1^\dagger + v b_1^\dagger\right)^J \left(a_1^\dagger b_L^\dagger - b_1^\dagger a_L^\dagger\right)^{S-J} \left(u a_L^\dagger + v b_L^\dagger\right)^J, \quad 0 \le J \le S. \tag{1.142}$$

These operators act on the direct product of Hilbert spaces of spins at site 1 and site L. Then the set of ground states of (1.141) can be chosen as

$$|\mathrm{G}; J, \hat{\Omega}\rangle \equiv A_J^\dagger |\mathrm{VBS}_L\rangle, \qquad J = 0, \ldots, S. \tag{1.143}$$

Any state $|\mathrm{G}; J, \hat{\Omega}\rangle$ of this set for fixed J and $\hat{\Omega}$ is a zero-energy ground state of (1.141). To prove this we need only to verify:

1. The total power of $a_1^\dagger$ and $b_1^\dagger$ is $2S$, so that we have spin-S at the first site;

2. The bond spin value satisfies $-S \leq J^z_{1,2} \equiv S^z_1 + S^z_2 \leq S$ by a binomial expansion, so that the maximum value of the bond spin $J_{1,2}$ is S (from $SU(2)$ invariance, see § 1.5.8 and [4]).

These properties are true for any other site j and bond $\langle j, j+1\rangle$, respectively. Therefore, the state $|\mathrm{G}; J, \hat{\Omega}\rangle$ defined in (1.143) has spin-S at each site and no projection onto the $J_{j,j+1} > S$ subspace for any bond.

Degenerate VBS States

The set of states $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ depend on a discrete parameter J as well as a continuous unit vector $\hat{\Omega}$. States with the same J value are not mutually orthogonal. It is possible also to introduce an orthogonal basis in description of the degenerate zero-energy ground states. This new basis could be used in determining the rank and the completeness of the set $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$. For notational convenience, we define

$$X_{JM} \equiv \frac{u^{J+M} v^{J-M}}{\sqrt{(J+M)!(J-M)!}}, \qquad \psi^\dagger_{Sm} \equiv \frac{(a^\dagger)^{S+m}(b^\dagger)^{S-m}}{\sqrt{(S+m)!(S-m)!}}. \quad (1.144)$$

These two variables transform conjugately with respect to one another under $SU(2)$. (See § 1.5.8 for more details of transformation properties.) Variable X_{JM} has the following orthogonality relation

$$\int \mathrm{d}\hat{\Omega} X^*_{JM} X_{JM'} = \frac{4\pi}{(2J+1)!}\delta_{MM'}. \quad (1.145)$$

Operator $\psi^\dagger_{Sm}$ is a spin state creation operator such that

$$\psi^\dagger_{Sm}|\mathrm{vac}\rangle = |S, m\rangle. \quad (1.146)$$

With the introduction of these variables (1.144), the operator $A^\dagger_J$ defined in (1.142) can be expanded as (see Chapter 9 of [25])

$$\begin{aligned} A^\dagger_J \;=\; & \sqrt{\frac{(S+J+1)!(S-J)!J!J!}{2J+1}} \\ & \cdot \sum_{M=-J}^{J} X_{JM} \sum_{m_1+m_L=M}^{m_1,m_L} (S/2, m_1; S/2, m_2|J, M)\; \psi^\dagger_{S/2,m_1} \otimes \psi^\dagger_{S/2,m_L}, \end{aligned} \quad (1.147)$$

where $(S/2, m_1; S/2, m_2|J, M)$ are the Clebsch-Gordan coefficients. Note that $\psi^\dagger_{S/2,m_1}$ and $\psi^\dagger_{S/2,m_L}$ are defined in the Hilbert spaces of spins at site 1 and site L, respectively. We realize that the particular form of the sum over m_1 and

m_L in (1.147) can be identified as a single spin state creation operator

$$\Psi^\dagger_{JM} \equiv \sum_{m_1,m_L}^{m_1+m_L=M} (S/2, m_1; S/2, m_2|J, M)\ \psi^\dagger_{S/2,m_1} \otimes \psi^\dagger_{S/2,m_L}. \tag{1.148}$$

This operator $\Psi^\dagger_{JM}$ acts on the direct product of two Hilbert spaces of spins at site 1 and site L. It has the property that

$$\Psi^\dagger_{JM}|\text{vac}\rangle_1 \otimes |\text{vac}\rangle_L = |J, M\rangle_{1,L}. \tag{1.149}$$

If we define a set of *degenerate VBS states* $\{|\text{VBS}_L(J, M)\rangle\}$ such that

$$|\text{VBS}_L(J, M)\rangle \equiv \Psi^\dagger_{JM}|\text{VBS}_L\rangle, \quad J = 0, ..., S, \quad M = -J, ..., J, \tag{1.150}$$

then these $(S + 1)^2$ states (1.150) are not only linearly independent but also mutually orthogonal.

The Orthogonality

To show the orthogonality of the degenerate VBS states (1.150), it is convenient to introduce the total spin operators of the subsystem (block):

$$S^+_{\text{tot}} = \sum_{j=1}^{L} a^\dagger_j b_j, \qquad S^-_{\text{tot}} = \sum_{j=1}^{L} b^\dagger_j a_j, \qquad S^z_{\text{tot}} = \frac{1}{2}\sum_{j=1}^{L}(a^\dagger_j a_j - b^\dagger_j b_j). \tag{1.151}$$

First we show that the set of operators $\{S^+_{\text{tot}}, S^-_{\text{tot}}, S^z_{\text{tot}}\}$ commute with the product of valence bonds, *i.e.*

$$[S^\pm_{\text{tot}}, \prod_{j=1}^{L-1}(a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] = 0, \quad [S^z_{\text{tot}}, \prod_{j=1}^{L-1}(a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] = 0. \tag{1.152}$$

These commutation relations (1.152) can be shown in similar ways. Take the commutator with $S^+_{\rm tot}$ first. We re-write the commutator as

$$
\begin{aligned}
& [S^+_{\rm tot}, \prod_{j=1}^{L-1} (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \qquad (1.153)\\
= & \sum_{j=1}^{L-1} (a^\dagger_1 b^\dagger_2 - b^\dagger_1 a^\dagger_2)^S \cdots [S^+_{\rm tot}, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \cdots (a^\dagger_{L-1} b^\dagger_L - b^\dagger_{L-1} a^\dagger_L)^S \\
= & \sum_{j=1}^{L-1} (a^\dagger_1 b^\dagger_2 - b^\dagger_1 a^\dagger_2)^S \cdots [S^+_j + S^+_{j+1}, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \cdots \\
& \cdots (a^\dagger_{L-1} b^\dagger_L - b^\dagger_{L-1} a^\dagger_L)^S .
\end{aligned}
$$

Then using commutators $[a_i, a^\dagger_j] = \delta_{ij}$ and $[b_i, b^\dagger_j] = \delta_{ij}$, we find that

$$
\begin{aligned}
& [S^+_j + S^+_{j+1}, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \\
= & [a^\dagger_j b_j + a^\dagger_{j+1} b_{j+1}, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \\
= & a^\dagger_j [b_j, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] + a^\dagger_{j+1} [b_{j+1}, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \\
= & a^\dagger_j (-S) a^\dagger_{j+1} (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^{S-1} + a^\dagger_{j+1} S a^\dagger_j (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^{S-1} \\
= & 0. \qquad (1.154)
\end{aligned}
$$

Therefore $[S^+_{\rm tot}, \prod_{j=1}^{L-1} (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] = 0$. In (1.154) we have used

$$
[b_j, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] = -S a^\dagger_{j+1} (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^{S-1}. \qquad (1.155)
$$

In a similar way, we find that the commutator with $S^-_{\rm tot}$ also vanishes. Next we consider the commutator with $S^z_{\rm tot}$:

$$
\begin{aligned}
& [S^z_{\rm tot}, \prod_{j=1}^{L-1} (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \qquad (1.156)\\
= & \sum_{j=1}^{L-1} (a^\dagger_1 b^\dagger_2 - b^\dagger_1 a^\dagger_2)^S \cdots [S^z_j + S^z_{j+1}, (a^\dagger_j b^\dagger_{j+1} - b^\dagger_j a^\dagger_{j+1})^S] \cdots \\
& \cdots (a^\dagger_{L-1} b^\dagger_L - b^\dagger_{L-1} a^\dagger_L)^S .
\end{aligned}
$$

In the right hand side of (1.156), the commutator involved also vanishes because

$$\begin{aligned}
& [S_j^z + S_{j+1}^z, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
= \; & \frac{1}{2}[a_j^\dagger a_j - b_j^\dagger b_j + a_{j+1}^\dagger a_{j+1} - b_{j+1}^\dagger b_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
= \; & a_j^\dagger [a_j, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] - b_j^\dagger [b_j, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
+ \; & a_{j+1}^\dagger [a_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] - b_{j+1}^\dagger [b_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
= \; & 0
\end{aligned} \tag{1.157}$$

Substituting (1.157) into (1.156), we obtain $[S_{\rm tot}^z, \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] = 0$. Now we shall show that the state $|{\rm VBS}_L(J,M)\rangle$ is a common eigenstate of $S_{\rm tot}^z$ and the total spin square $\boldsymbol{S}_{\rm tot}^2 = \frac{1}{2}(S_{\rm tot}^+ S_{\rm tot}^- + S_{\rm tot}^- S_{\rm tot}^+) + (S_{\rm tot}^z)^2$ with eigenvalues M and $J(J+1)$, respectively. Using the commutation relations (1.152), we can show that

$$\begin{aligned}
S_{\rm tot}^\pm |{\rm VBS}_L(J,M)\rangle &= \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S (S_1^\pm + S_L^\pm)|J,M\rangle_{1,L}|{\rm vac}\rangle_{2,\ldots,L-1} \\
S_{\rm tot}^z |{\rm VBS}_L(J,M)\rangle &= \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S (S_1^z + S_L^z)|J,M\rangle_{1,L}|{\rm vac}\rangle_{2,\ldots,L-1}.
\end{aligned} \tag{1.158}$$

Then from the definition of the state $|{\rm VBS}_L(J,M)\rangle$ and the following relations:

$$\begin{aligned}
(S_1^+ + S_L^+)|J,M\rangle_{1,L} &= \sqrt{(J \mp M)(J \pm M + 1)}\; |J, M \pm 1\rangle, \\
(S_1^z + S_L^z)|J,M\rangle_{1,L} &= M|J,M\rangle_{1,L},
\end{aligned} \tag{1.159}$$

we obtain

$$\begin{aligned}
S_{\rm tot}^\pm |{\rm VBS}_L(J,M)\rangle &= \sqrt{(J \mp M)(J \pm M + 1)}\; |{\rm VBS}_L(J, M \pm 1)\rangle, \\
S_{\rm tot}^z |{\rm VBS}_L(J,M)\rangle &= M|{\rm VBS}_L(J,M)\rangle
\end{aligned} \tag{1.160}$$

and hence $\boldsymbol{S}_{\rm tot}^2 |{\rm VBS}_L(J,M)\rangle = J(J+1)|{\rm VBS}_L(J,M)\rangle$. It is now proved that $|{\rm VBS}_L(J,M)\rangle$ is a common eigenstate of Hermitian operators $S_{\rm tot}^z$ and $\boldsymbol{S}_{\rm tot}^2$ with eigenvalues M and $J(J+1)$, respectively. Therefore the states with different eigenvalues (J,M) are orthogonal to each other. Thus we have proved the orthogonality of the set $\{|{\rm VBS}_L(J,M)\rangle \mid J = 0, \ldots, S;\; M = -J, \ldots, J\}$.

Completeness and Equivalence

It is obvious from (1.147) that any ground state $|\mathrm{G};J,\hat{\Omega}\rangle$ can be written as a linear superposition over these degenerate VBS states:

$$|\mathrm{G};J,\hat{\Omega}\rangle = \sqrt{\frac{(S+J+1)!(S-J)!J!J!}{2J+1}} \sum_{M=-J}^{J} X_{JM}|\mathrm{VBS}_L(J,M)\rangle, \quad (1.161)$$

and *vice versa*. Now we can derive the completeness relation of the set $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ using (1.145), (1.147) and (1.148):

$$\begin{aligned} &\int \mathrm{d}\hat{\Omega}|\mathrm{G};J,\hat{\Omega}\rangle\langle\mathrm{G};J,\hat{\Omega}| \quad (1.162)\\ = \;& \frac{4\pi}{(2J+1)!}\frac{(S+J+1)!(S-J)!J!J!}{2J+1} \sum_{M=-J}^{J} \Psi_{JM}^{\dagger}|\mathrm{VBS}_L\rangle\langle\mathrm{VBS}_L|\Psi_{JM}. \end{aligned}$$

The set of states $\{\Psi_{JM}^{\dagger}|\mathrm{VBS}_L\rangle \mid M=-J,\ldots,J\}$ are linearly independent. So that the rank of $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ with fixed J value is $2J+1$, which can be obtained from the completeness relation (1.162) (see [25]). Thus the total number of linearly independent states of the set $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ is $\sum_{J=0}^{S}(2J+1) = (S+1)^2$, which is exactly the degeneracy of the ground states of (1.141). So that $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ forms a complete set of zero-energy ground states. The set $\{|\mathrm{VBS}_L(J,M)\rangle\}$ differs from $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ by a change of basis, therefore it also forms a complete set of zero-energy ground states. These two sets (1.143) and (1.150) are equivalent in description of the degenerate ground states of the block Hamiltonian (1.141). (More details such as the expansion (1.147) *etc.* can be found in Chapter 9 of [25].)

1.5.4 Eigenvectors of the Density Matrix

Eigenvalues of the density matrix $\boldsymbol{\rho}_L$ can be derived indirectly, as in [11] for spin-1 (see § 1.4.4 for comparison) and in [32] for spin-S. The basic idea is the following: Because the density matrix is independent of both the total length of the spin chain and the starting site of the block, we can add boundary spins directly to the ends of the block. It was shown in [11, 32] by a Schmidt decomposition (see Section 2.5 of [41]) that non-zero eigenvalues of the density matrix (1.138) are equal to those of the density matrix of the two boundary spins. All other eigenvalues of the density matrix (1.138) are zero. This fact reveals the structure of the density matrix as a projector (up to a multiplicative 'scaling' matrix) onto a subspace of dimension $(S+1)^2$.

Now we propose a theorem on the eigenvectors of the density matrix $\boldsymbol{\rho}_L$ given by (1.138). The explicit construction of eigenvectors allows us to diagonalize the density matrix directly. The set of eigenvectors also spans the subspace that the density matrix projects onto.

Theorem 1.2

Eigenvectors of the density matrix $\boldsymbol{\rho}_L$ (1.138) with non-zero eigenvalues are given by the set $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ (1.143), or, equivalently, by the set $\{|\mathrm{VBS}_L(J, M)\rangle\}$ (1.150). *i.e.* They are zero-energy ground states of the block Hamiltonian H_B (1.141).

We prove this theorem by showing that the density matrix $\boldsymbol{\rho}_L$ (1.138) can be written as a projector in diagonal form onto the orthogonal degenerate VBS states $\{|\mathrm{VBS}_L(J, M)\rangle\}$ introduced in (1.150). An alternative proof taking a different approach is given in the next section § 1.5.5 .

First, it is realized from the definition of spinor coordinates (1.120) that if we change variables (u, v) to $(\mathrm{i}v^*, -\mathrm{i}u^*)$, then the unit vector $\hat{\Omega}$ is inverted about the origin to $-\hat{\Omega}$. So that we have [32]

$$(u^* b^\dagger - v^* a^\dagger)^S |\mathrm{vac}\rangle = \mathrm{i}^S \sqrt{S!}\, |-\hat{\Omega}\rangle, \tag{1.163}$$

where $|-\hat{\Omega}\rangle$ means a spin-$S/2$ coherent state for a point opposite to $\hat{\Omega}$ on the unit sphere. Therefore, taking expressions of the boundary operator $B^\dagger$ (1.139) and the block VBS state $|\mathrm{VBS}_L\rangle$ (1.140), we have

$$\begin{aligned} &B^\dagger |\mathrm{VBS}_L\rangle = \\ &S! \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger \right)^S |-\hat{\Omega}_0\rangle_1 \otimes |\mathrm{vac}\rangle_2 \otimes \cdots \otimes |\mathrm{vac}\rangle_{L-1} \otimes |-\hat{\Omega}_{L+1}\rangle_L . \end{aligned} \tag{1.164}$$

Consequently the density matrix $\boldsymbol{\rho}_L$ (1.138) can be re-written as

$$\begin{aligned} \boldsymbol{\rho}_L \quad &= \left[\frac{S+1}{(2S+1)!} \right]^L \frac{S!S!}{S+1} \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger \right)^S \\ &\cdot I_{S+1}^{(1)} \otimes |\mathrm{vac}\rangle_2 \langle \mathrm{vac}| \otimes \cdots \otimes |\mathrm{vac}\rangle_{L-1} \langle \mathrm{vac}| \otimes I_{S+1}^{(L)} \prod_{j=1}^{L-1} \left(a_j b_{j+1} - b_j a_{j+1} \right)^S , \end{aligned} \tag{1.165}$$

where $I_{S+1}^{(1)}$ and $I_{S+1}^{(L)}$ are $(S+1)$-dimensional identities associated with site 1 and site L, respectively. In obtaining (1.165), we have changed integral variables from $\hat{\Omega}_0$, $\hat{\Omega}_{L+1}$ to $-\hat{\Omega}_0$, $-\hat{\Omega}_{L+1}$ and performed these two integrals

using the completeness relation (1.122). Next we notice that (see § 1.5.3)

$$
\begin{aligned}
I^{(1)}_{S+1} \otimes I^{(L)}_{S+1} &= \sum_{J=0}^{S} \sum_{M=-J}^{J} |J,M\rangle_{1,L}\langle J,M| \qquad (1.166)\\
&= \sum_{J=0}^{S} \sum_{M=-J}^{J} \Psi^{\dagger}_{JM} |\mathrm{vac}\rangle_1\langle \mathrm{vac}| \otimes |\mathrm{vac}\rangle_L\langle \mathrm{vac}| \Psi_{JM}.
\end{aligned}
$$

As a result, combining (1.165) and (1.166), recalling definitions of $|\mathrm{VBS}_L\rangle$ (1.140) and $|\mathrm{VBS}_L(J,M)\rangle$ (1.150), the density matrix $\boldsymbol{\rho}_L$ takes the following final form

$$
\begin{aligned}
\boldsymbol{\rho}_L &= \left[\frac{S+1}{(2S+1)!}\right]^L \frac{S!S!}{S+1} \sum_{J=0}^{S} \sum_{M=-J}^{J} \Psi^{\dagger}_{JM} |\mathrm{VBS}_L\rangle\langle \mathrm{VBS}_L| \Psi_{JM} \qquad (1.167)\\
&= \left[\frac{S+1}{(2S+1)!}\right]^L \frac{S!S!}{S+1} \sum_{J=0}^{S} \sum_{M=-J}^{J} |\mathrm{VBS}_L(J,M)\rangle\langle \mathrm{VBS}_L(J,M)|.
\end{aligned}
$$

The set of degenerate VBS states $\{|\mathrm{VBS}_L(J,M)\rangle\}$ with $J = 0,\ldots,S$ and $M = -J,\ldots,J$ forms an orthogonal basis (see § 1.5.3). These $(S+1)^2$ states also forms a complete set of zero-energy ground states of the block Hamiltonian (1.141) (see § 1.5.3). So that in expression (1.167) we have put the density matrix as a projector in diagonal form over an orthogonal basis. Each degenerate VBS state $|\mathrm{VBS}_L(J,M)\rangle$ is an eigenvector of the density matrix, so as any of the state $|\mathrm{G};J,\hat{\Omega}\rangle$ (because of the degeneracy of corresponding eigenvalues of the density matrix, see § 1.5.6 and § 1.5.7 that the eigenvalues depend only on J). Thus we have proved **Theorem 1.2**.

1.5.5 An Alternative Proof of Theorem 1.2

It was shown in § 1.5.4 that the density matrix takes a diagonal form in the basis of zero-energy ground states of the block Hamiltonian (1.141). In this section, we show the same result by taking a different approach. This alternative proof of **Theorem 1.2** does not involve the coherent state basis.

The proof uses the fact that the density matrix is independent of the starting site and the total length of the chain (see § 1.5.2). So that we could change the configuration of the whole system by adding the two ending spins directly to the block without affecting the form of the block density matrix. The new system now has $L+2$ sites with the block starting at site 1 and ending at site L. Let us start with the ground VBS state of the Hamiltonian (1.116) of the

system with $N = L$:

$$|\mathrm{VBS}\rangle \equiv \prod_{j=0}^{L} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger \right)^S |\mathrm{vac}\rangle. \tag{1.168}$$

In order to calculate the density matrix $\boldsymbol{\rho}_L = \mathrm{tr}_{0,L+1}[\,\boldsymbol{\rho}\,]$, where $\boldsymbol{\rho}$ is defined in (1.119), we introduce a useful identity:

$$ {}_{0,L+1}\langle J, M| \left(|s\rangle_{0,1} \otimes |s\rangle_{L,L+1} \right) = \frac{(-1)^{S-J+M}}{(S+1)} |J, -M\rangle_{1,L}, \tag{1.169}$$

where $|J, M\rangle_{0,L+1}$ is identical to the spin state defined in (1.149) except for site indices. $|s\rangle_{i,j}$ in (1.169) is the normalized singlet state with S valence bonds defined as

$$\begin{aligned} |s\rangle_{i,j} &= \frac{1}{S!\sqrt{S+1}} \left(a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger \right)^S |\mathrm{vac}\rangle_i \otimes |\mathrm{vac}\rangle_j \\ &= \frac{(-1)^{\frac{S}{2}}}{\sqrt{S+1}} \sum_{m=-S/2}^{S/2} (-1)^m |S/2, -m\rangle_i \otimes |S/2, m\rangle_j. \end{aligned} \tag{1.170}$$

Identity (1.169) is derived using properties of the singlet state (1.170) and Clebsch-Gordan coefficients as follows:

$$\begin{aligned} & {}_{0,L+1}\langle J, M| \left(|s\rangle_{0,1} \otimes |s\rangle_{L,L+1} \right) \\ = & \sum_{m_0, m_{L+1}}^{m_0+m_{L+1}=M} (J, M|S/2, m_0; S/2, m_{L+1}) {}_0\langle S/2, m_0|_{L+1}\langle S/2, m_{L+1}| \\ \cdot & \frac{(-1)^{\frac{S}{2}}}{\sqrt{S+1}} \sum_{m_1=-S/2}^{S/2} (-1)^{m_1} |S/2, -m_1\rangle_0 |S/2, m_1\rangle_1 \\ \cdot & \frac{(-1)^{\frac{S}{2}}}{\sqrt{S+1}} \sum_{m_L=-S/2}^{S/2} (-1)^{m_L} |S/2, -m_L\rangle_L |S/2, m_L\rangle_{L+1} \\ = & \frac{1}{S+1} \sum_{m_0, m_{L+1}}^{m_0+m_{L+1}=M} (-1)^{m_0+m_{L+1}} (J, M|S/2, m_0; S/2, m_{L+1}) \\ \cdot & |S/2, -m_0\rangle_1 |S/2, -m_{L+1}\rangle_L. \end{aligned} \tag{1.171}$$

Here the Clebsch-Gordan coefficient is defined by

$$(J, M|S/2, m_0; S/2, m_{L+1}) = {}_{i,j}\langle J, M| \left(|S/2, m_0\rangle_i \otimes |S/2, m_{L+1}\rangle_j\right). \quad (1.172)$$

Then using the symmetry property of Clebsch-Gordan coefficients

$$(J, M|S/2, m_0; S/2, m_{L+1}) = (-1)^{S-J}(J, -M|S/2, -m_0; S/2, -m_{L+1}), \quad (1.173)$$

and the completeness of the basis $\{|S/2, m_0\rangle_0 \otimes |S/2, m_{L+1}\rangle_{L+1}\}$, we obtain the identity (1.169).

With the help of identity (1.169), we calculate the partial inner product of the VBS state (1.168) with the state $|J, M\rangle_{0,L+1}$, which is involved in taking trace of boundary spins. The VBS state $|\mathrm{VBS}\rangle$ is decomposed into the bulk part and boundary parts, then making use of (1.169), we have

$$\begin{aligned}
& {}_{0,L+1}\langle J, M|\mathrm{VBS}\rangle \\
= \; & {}_{0,L+1}\langle J, M| \prod_{j=0}^{L} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\mathrm{vac}\rangle \\
= \; & S!(S+1)! \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S {}_{0,L+1}\langle J, M|s\rangle_{0,1}|s\rangle_{L,L+1}|\mathrm{vac}\rangle_{2\cdots L-1} \\
= \; & (S!)^2 \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S (-1)^{S-J+M}|J, -M\rangle_{1,L}|\mathrm{vac}\rangle_{2\cdots L-1} \\
= \; & (-1)^{S-J+M}(S!)^2|\mathrm{VBS}_L(J, -M)\rangle. \quad (1.174)
\end{aligned}$$

We see that the $(S+1)^2$ degenerate VBS states $\{|\mathrm{VBS}_L(J, M)\rangle\}$ defined in (1.150) appear in the partial inner product (1.174). As discussed in § 1.5.3 , they form a complete set of zero-energy ground states of the block Hamiltonian (1.141).

Now, it is straightforward to evaluate the density matrix as

$$\begin{aligned}
\mathrm{tr}_{0,L+1}[\,\boldsymbol{\rho}\,] &= \sum_{J,M} \frac{{}_{0,L+1}\langle J, M|\mathrm{VBS}\rangle\langle\mathrm{VBS}|J, M\rangle_{0,L+1}}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle} \\
&= \frac{(S!)^4}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle} \sum_{J,M} |\mathrm{VBS}_L(J, -M)\rangle\langle\mathrm{VBS}_L(J, -M)|.
\end{aligned} \quad (1.175)$$

This expression is identical to (1.167) as we change dummy index from M to $-M$. Therefore, in this approach again we arrive at **Theorem 1.2** that the density matrix is proportional to a projector onto a subspace spanned by the $(S+1)^2$ ground states of the block Hamiltonian (1.141). Normalization $\langle \mathrm{VBS}|\mathrm{VBS}\rangle$ has been obtained in § 1.5.1 . States $|\mathrm{VBS}_L(J,M)\rangle$ have been shown to be mutually orthogonal in § 1.5.3 .

1.5.6 Eigenvalues of the Density Matrix (Normalization of Degenerate VBS States)

As the next step in analyzing the spectrum of the density matrix, now we study the eigenvalues. Based on the diagonalized form (1.167), it is clear that eigenvalues of the density matrix $\boldsymbol{\rho}_L$ can be derived from the normalization of degenerate VBS states. We obtain an explicit expression for eigenvalues in terms of Wigner $3j$-symbols in this section.

First, the following property is important: Normalization of the degenerate VBS state $|\mathrm{VBS}_L(J,M)\rangle$ depends only on J and is independent of M. This point is important in proving that any $|\mathrm{G};J,\hat{\Omega}\rangle$ is an eigenvector of $\boldsymbol{\rho}_L$ because it can be written as a superposition of $|\mathrm{VBS}_L(J,M)\rangle$'s with the same J value (1.161). With the introduction of total spin operators of the block $S^{\pm}_{\mathrm{tot}}$, S^{z}_{tot} and $\boldsymbol{S}^2_{\mathrm{tot}}$ (see § 1.5.3), we prove the statement as follows:

$$\begin{aligned}
& \langle \mathrm{VBS}_L(J,M\pm 1)|\mathrm{VBS}_L(J,M\pm 1)\rangle \\
= \; & \frac{1}{(J\mp M)(J\pm M+1)}\langle \mathrm{VBS}_L(J,M)|S^{\mp}_{\mathrm{tot}}S^{\pm}_{\mathrm{tot}}|\mathrm{VBS}_L(J,M)\rangle \\
= \; & \frac{1}{(J\mp M)(J\pm M+1)}\langle \mathrm{VBS}_L(J,M)|(\boldsymbol{S}^2_{\mathrm{tot}}-(S^{z}_{\mathrm{tot}})^2\mp S^{z}_{\mathrm{tot}})|\mathrm{VBS}_L(J,M)\rangle \\
= \; & \langle \mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle. \qquad (1.176)
\end{aligned}$$

Here we have used the fact that $|\mathrm{VBS}_L(J,M)\rangle$ is the common eigenstate of $\boldsymbol{S}^2_{\mathrm{tot}}$ and S^{z}_{tot} with eigenvalues $J(J+1)$ and M, respectively (see § 1.5.3).

It is also realized that the normalization of $|\mathrm{VBS}_L(J,M)\rangle$ can be calculated from integrating the inner product of $|\mathrm{G};J,\hat{\Omega}\rangle$ with itself over the unit vector $\hat{\Omega}$ such that

$$\begin{aligned}
& \frac{1}{4\pi}\int \mathrm{d}\hat{\Omega}\langle \mathrm{G};J,\hat{\Omega}|\mathrm{G};J,\hat{\Omega}\rangle \\
= \; & \frac{(S+J+1)!(S-J)!J!J!}{(2J+1)!}\langle \mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle. \qquad (1.177)
\end{aligned}$$

In obtaining this relation (1.177) we have used expansion (1.161) and orthog-

onality (1.145) in § 1.5.3 .

Let us consider the integral involved in (1.177). Using the coherent state basis (1.121) and completeness relation (1.122) as before, we obtain

$$\begin{aligned} & \frac{1}{4\pi}\int \mathrm{d}\hat{\Omega}\langle \mathrm{G};J,\hat{\Omega}|\mathrm{G};J,\hat{\Omega}\rangle \qquad (1.178)\\ = \; & \frac{1}{4\pi}\left[\frac{(2S+1)!}{4\pi}\right]^{L}\int \mathrm{d}\hat{\Omega}\int\left[\prod_{j=1}^{L}\mathrm{d}\hat{\Omega}_j\right]\prod_{j=1}^{L-1}\left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^{S}\\ \cdot \; & \left[\frac{1}{2}(1-\hat{\Omega}_1\cdot\hat{\Omega}_L)\right]^{S-J}\left[\frac{1}{2}(1+\hat{\Omega}_1\cdot\hat{\Omega})\right]^{J}\left[\frac{1}{2}(1+\hat{\Omega}\cdot\hat{\Omega}_L)\right]^{J}. \end{aligned}$$

Now we expand $\left[\frac{1}{2}(1-\hat{\Omega}_i\cdot\hat{\Omega}_j)\right]^{J}$ in terms of spherical harmonics as in (1.130), then integrate over $\hat{\Omega}$ and from $\hat{\Omega}_2$ to $\hat{\Omega}_{L-1}$, the right hand side of (1.178) is equal to

$$\begin{aligned} & \frac{4\pi((2S+1)!)^{L}}{(S+1)^{L-1}(S-J+1)(J+1)^{2}}\sum_{l_1=0}^{S}\sum_{l_L=0}^{S-J}\sum_{l=0}^{J}\sum_{m_1=-l_1}^{l_1}\sum_{m_L=-l_L}^{l_L}\sum_{m=-l}^{l}\\ \cdot \; & \int \mathrm{d}\hat{\Omega}_1\int \mathrm{d}\hat{\Omega}_L\lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\lambda^{2}(l,J)\\ \cdot \; & Y_{l_1,m_1}(\hat{\Omega}_1)Y_{l_L,m_L}(\hat{\Omega}_1)Y_{l,m}(\hat{\Omega}_1)Y^{*}_{l_1,m_1}(\hat{\Omega}_L)Y^{*}_{l_L,m_L}(\hat{\Omega}_L)Y^{*}_{l,m}(\hat{\Omega}_L). \qquad (1.179) \end{aligned}$$

Here we apply the following useful formula:

$$\begin{aligned} & \int \mathrm{d}\hat{\Omega}Y_{l_1,m_1}(\hat{\Omega})Y_{l_L,m_L}(\hat{\Omega})Y_{l,m}(\hat{\Omega})\\ = \; & \sqrt{\frac{(2l_1+1)(2l_L+1)(2l+1)}{4\pi}}\begin{pmatrix} l_1 & l_L & l\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_1 & l_L & l\\ m_1 & m_L & m\end{pmatrix}, \qquad (1.180) \end{aligned}$$

where $\begin{pmatrix} l_1 & l_L & l\\ m_1 & m_L & m\end{pmatrix}$ is the Wigner $3j$-symbol. Using formula (1.180), we

carry out the remaining integrals in (1.179) and obtain

$$\frac{((2S+1)!)^L}{(S+1)^{L-1}(S-J+1)(J+1)^2}\sum_{l_1=0}^{S}\sum_{l_L=0}^{S-J}\sum_{l=0}^{J}\sum_{m_1=-l_1}^{l_1}\sum_{m_L=-l_L}^{l_L}\sum_{m=-l}^{l}$$
$$\cdot\ (2l_1+1)(2l_L+1)(2l+1)\lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\lambda^2(l,J)$$
$$\cdot\ \begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{pmatrix} l_1 & l_L & l \\ m_1 & m_L & m \end{pmatrix}^2. \tag{1.181}$$

These $3j$-symbols obey the following orthogonality relation:

$$\sum_{m_1,m_L}(2l+1)\begin{pmatrix} l_1 & l_L & l \\ m_1 & m_L & m \end{pmatrix}\begin{pmatrix} l_1 & l_L & l' \\ m_1 & m_L & m' \end{pmatrix} = \delta_{ll'}\delta_{mm'}. \tag{1.182}$$

Using this orthogonality (1.182), we can recast expression (1.181) as

$$\frac{((2S+1)!)^L}{(S+1)^{L-1}(S-J+1)(J+1)^2}\sum_{l_1=0}^{S}\sum_{l_L=0}^{S-J}\sum_{l=0}^{J} \tag{1.183}$$
$$\cdot\ (2l_1+1)(2l_L+1)(2l+1)\lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\lambda^2(l,J)\begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}^2.$$

The explicit value of $\begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}$ is given by

$$\begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}$$
$$= (-1)^g\sqrt{\frac{(2g-2l_1)!(2g-2l_L)!(2g-2l)!}{(2g+1)!}}\frac{g!}{(g-l_1)!(g-l_L)!(g-l)!}, \tag{1.184}$$

if $l_1+l_L+l=2g$ ($g\in\mathbf{N}$), otherwise zero. Finally, the normalization of degenerate VBS states $|\mathrm{VBS}_L(J,M)\rangle$ is obtained as

$$\langle\mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle \tag{1.185}$$
$$= \frac{(2J+1)!((2S+1)!)^L}{(S+1)^{L-1}(S+J+1)!(S-J+1)!(J+1)!(J+1)!}\sum_{l_1=0}^{S}\sum_{l_L=0}^{S-J}\sum_{l=0}^{J}$$
$$(2l_1+1)(2l_L+1)(2l+1)\lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\lambda^2(l,J)\begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}^2.$$

Combining results of (1.167) and (1.185), we arrive at the following theorem on eigenvalues:

Theorem 1.3

Eigenvalues $\Lambda(J)$ $(J = 0, \ldots, S)$ of the density matrix $\boldsymbol{\rho}_L$ are independent of $\hat{\Omega}$ and M in defining eigenvectors (see (1.143) and (1.150)). An explicit expression is given by the following triple sum

$$\begin{aligned} & \Lambda(J) \qquad\qquad (1.186) \\ = & \left[\frac{S+1}{(2S+1)!}\right]^L \frac{S!S!}{S+1} \langle \mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle \\ = & \frac{(2J+1)!S!S!}{(S+J+1)!(S-J+1)!(J+1)!(J+1)!} \sum_{l_1=0}^{S} \sum_{l_L=0}^{S-J} \sum_{l=0}^{J} \\ & \cdot(2l_1+1)(2l_L+1)(2l+1)\lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\lambda^2(l,J) \begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}^2 . \end{aligned}$$

Although not straightforward to verify, this expression (1.186) should be consistent with eigenvalues given through the recurrence expression (1.199) in the next section § 1.5.7 and the expression Λ_α in § 1.4.4 as a special case. We could check the case when $S = 1$ that

$$\begin{aligned} \langle \mathrm{VBS}_L(0,0)|\mathrm{VBS}_L(0,0)\rangle &= \frac{1}{2}(3^L + 3(-1)^L), \\ \langle \mathrm{VBS}_L(1,M)|\mathrm{VBS}_L(1,M)\rangle &= \frac{1}{2}(3^L - (-1)^L), \end{aligned} \qquad (1.187)$$

where we have used the selection rule of the Wigner $3j$-symbol. From (1.133) we find that $\langle \mathrm{VBS}|\mathrm{VBS}\rangle = 2 \cdot 3^L$, so that we obtain the correct eigenvalues of the density matrix from the above result (1.186) (see § 1.4.4 for comparison).

We shall emphasize at this point that given eigenvalues (1.186), both von Neumann entropy

$$S_{\mathrm{v\ N}} = -\mathrm{tr}\,[\,\boldsymbol{\rho}_L \ln \boldsymbol{\rho}_L\,] = -\sum_{J=0}^{S}(2J+1)\Lambda(J)\ln\Lambda(J) \qquad (1.188)$$

and Rényi entropy

$$S_R = \frac{1}{1-\alpha}\ln\{\mathrm{tr}\,[\,\boldsymbol{\rho}_L^\alpha\,]\} = \frac{1}{1-\alpha}\ln\left\{\sum_{J=0}^{S}(2J+1)\Lambda^\alpha(J)\right\} \qquad (1.189)$$

can be expressed directly.

1.5.7 Eigenvalues of the Density Matrix (Recurrence Formula)

Having constructed eigenvectors, there are more than one way to specify the corresponding eigenvalues. An explicit expression of eigenvalues has been obtained in § 1.5.6 . In this section we express eigenvalues through a conjectured recurrence formula as appeared in [18, 32]. Let us apply the density matrix $\boldsymbol{\rho}_L$ (1.138) to the state $|\mathrm{G}; J, \hat{\Omega}\rangle$ (1.143) and obtain

$$\begin{aligned} & \boldsymbol{\rho}_L|\mathrm{G}; J, \hat{\Omega}\rangle \\ = & \left[\frac{S+1}{(2S+1)!}\right]^L \frac{S+1}{(4\pi)^2} \int \mathrm{d}\hat{\Omega}_0 \mathrm{d}\hat{\Omega}_{L+1} B^\dagger |\mathrm{VBS}_L\rangle\langle \mathrm{VBS}_L| B A_J^\dagger |\mathrm{VBS}_L\rangle. \end{aligned} \tag{1.190}$$

Using the coherent state basis (1.121) and completeness relation (1.122), the factor $\langle \mathrm{VBS}_L| B A_J^\dagger |\mathrm{VBS}_L\rangle$ in (1.190) can be re-written as

$$\begin{aligned} & \langle \mathrm{VBS}_L| B A_J^\dagger |\mathrm{VBS}_L\rangle \\ = & \left[\frac{(2S+1)!}{4\pi}\right]^L \int \left(\prod_{j=1}^{L} \mathrm{d}\hat{\Omega}_j\right) \prod_{j=1}^{L-1} \left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S (u_0 v_1 - v_0 u_1)^S \\ & \cdot (u u_1^* + v v_1^*)^J (u_1^* v_L^* - v_1^* u_L^*)^{S-J} (u u_L^* + v v_L^*)^J (u_L v_{L+1} - v_L u_{L+1})^S . \end{aligned} \tag{1.191}$$

The factor $\left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S$ under the integral of (1.191) can be expanded in terms of Legendre polynomials and further in terms of spherical harmonics as discussed in § 1.5.1 (see also [18, 32]). Using the expansion (1.130) and orthogonality of spherical harmonics, the integrals over $\hat{\Omega}_j$ with $j = 2, \ldots, L-1$ in (1.191) can be performed. The result is

$$\begin{aligned} \langle \mathrm{VBS}_L| B A_J^\dagger |\mathrm{VBS}_L\rangle \quad = & \frac{S+1}{(4\pi)^2} \left[\frac{(2S+1)!}{S+1}\right]^L \sum_{l=0}^{S} (2l+1)\lambda^{L-1}(l,S) \\ & \cdot \int \mathrm{d}\hat{\Omega}_1 \mathrm{d}\hat{\Omega}_L P_l(\hat{\Omega}_1\cdot\hat{\Omega}_L) (u_0 v_1 - v_0 u_1)^S (u u_1^* + v v_1^*)^J \\ & (u_1^* v_L^* - v_1^* u_L^*)^{S-J} (u u_L^* + v v_L^*)^J (u_L v_{L+1} - v_L u_{L+1})^S . \end{aligned} \tag{1.192}$$

We plug the expression (1.192) into (1.190). Using transformation properties under $SU(2)$ and a binomial expansion (see § 1.5.8), the integral over $\hat{\Omega}_0$ yields

that

$$\int \mathrm{d}\hat{\Omega}_0 \left(u_0^* b_1^\dagger - v_0^* a_1^\dagger\right)^S (u_0 v_1 - v_0 u_1)^S = \frac{4\pi}{S+1}\left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^S \quad (1.193)$$

Similarly we can perform the integral over $\hat{\Omega}_{L+1}$. As a result, the following expression is obtained from (1.190):

$$\boldsymbol{\rho}_L|\mathrm{G}; J, \hat{\Omega}\rangle = \frac{1}{(4\pi)^2}\sum_{l=0}^{S}(2l+1)\lambda^{L-1}(l,S)K_l^\dagger(\hat{\Omega})\,|\mathrm{VBS}_L\rangle\,. \quad (1.194)$$

The operator $K_l^\dagger(\hat{\Omega})$ involved in (1.194) is defined as

$$\begin{aligned} K_l^\dagger(\hat{\Omega}) \;\equiv\; & \int \mathrm{d}\hat{\Omega}_1 \mathrm{d}\hat{\Omega}_L \left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^S (u u_1^* + v v_1^*)^J (u_1^* v_L^* - v_1^* u_L^*)^{S-J} \\ & \cdot (u u_L^* + v v_L^*)^J \left(u_L a_L^\dagger + v_L b_L^\dagger\right)^S P_l(\hat{\Omega}_1 \cdot \hat{\Omega}_L). \end{aligned} \quad (1.195)$$

It is expressed as an integral depending on the order l of the Legendre polynomial $P_l(\hat{\Omega}_1 \cdot \hat{\Omega}_L)$. $K_l^\dagger(\hat{\Omega})$ can be calculated from the lowest few orders (see § 1.5.8 for example). It becomes increasingly difficult to perform the integral as order l increases. Based on the eigenvalue expressions of the density matrix obtained in [11, 32], we make a conjecture on the explicit form of the operator $K_l^\dagger(\hat{\Omega})$ for generic order l:

Conjecture 1.1

$$K_l^\dagger(\hat{\Omega}) = \left(\frac{4\pi}{S+1}\right)^2 I_l\left(\frac{1}{2}J(J+1) - \frac{1}{2}S(\frac{1}{2}S+1)\right) A_J^\dagger. \quad (1.196)$$

Here the polynomial $I_l\,(x)$ satisfy the recurrence relation

$$I_{l+1}(x) = \frac{2l+1}{(S+l+2)^2}\left(\frac{4x}{l+1}+l\right) I_l\,(x) - \frac{l}{l+1}\left(\frac{S-l+1}{S+l+2}\right)^2 I_{l-1}(x) \quad (1.197)$$

with $I_0 = 1$ and $I_1 = \frac{x}{(\frac{S}{2}+1)^2}$.

Note that it is important that $K_l^\dagger(\hat{\Omega}) \propto A_J^\dagger$ defined in (1.142) and $I_l(x)$ has the same order as the Legendre polynomial $P_l(x)$. The recurrence relation (1.197) was proposed in [18] and used in [32] to obtain the eigenvalues of the density matrix. (The original definition of $I_l(x)$ differs from our definition in (1.197) by a factor of $\frac{2l+1}{4\pi}$.) **Conjecture 1.1** is an alternative form of **The-**

orem 1.2 together with **Theorem 1.3**, which also gives eigenvalues through the recurrence relation (1.197). Indeed, expressions (1.194), altogether with (1.196) and (1.197) yields that

$$\begin{aligned} & \boldsymbol{\rho}_L|\mathrm{G};J,\hat{\Omega}\rangle \qquad (1.198)\\ = & \frac{1}{(S+1)^2}\sum_{l=0}^{S}(2l+1)\lambda^{L-1}(l,S)I_l\left(\frac{1}{2}J(J+1)-\frac{1}{2}S(\frac{1}{2}S+1)\right)|\mathrm{G};J,\hat{\Omega}\rangle. \end{aligned}$$

Non-zero eigenvalues ($J=0,1,\ldots,S$) are seen from (1.198) as

$$\Lambda(J)\equiv\frac{1}{(S+1)^2}\sum_{l=0}^{S}(2l+1)\lambda^{L-1}(l,S)I_l\left(\frac{1}{2}J(J+1)-\frac{1}{2}S(\frac{1}{2}S+1)\right). \qquad (1.199)$$

Since all other eigenvalues of the density matrix are vanishing, then we conclude again that the density matrix $\boldsymbol{\rho}_L$ (1.138) is a projector onto a subspace of dimension $(S+1)^2$. This subspace is spanned by the set of vectors $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ (1.143). (The rank of the set is equal to $(S+1)^2$.) Furthermore, we observe from (1.199) again that non-zero eigenvalues $\Lambda(J)$ depend only on J, not on $\hat{\Omega}$. Therefore, $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ with fixed J value spans a degenerate subspace with the same eigenvalue.

1.5.8 The Large Block Limit

In the limit $L\to\infty$, that is when the size of the block becomes large, we learned from [11, 21, 32] that the von Neumann entropy reaches the saturated value $S_{\mathrm{v\ N}}=\ln(S+1)^2$. This fact implies that the density matrix (denoted by $\boldsymbol{\rho}_\infty$ in the limit) can only take the form (see [41] for a general proof)

$$\boldsymbol{\rho}_\infty=\frac{1}{(S+1)^2}I_{(S+1)^2}\oplus\Phi_\infty, \qquad (1.200)$$

where $I_{(S+1)^2}$ is the identity of dimension $(S+1)^2$ and Φ_∞ is an infinite dimensional matrix with only zero entries. In this section, we give a proof of **Conjecture 1.1** (1.196) in the limiting case as $L\to\infty$. Then we shall verify the structure of the density matrix (1.200) explicitly.

We first realize from (1.131) that as $L\to\infty$, $\lambda^{L-1}(l,S)\to\delta_{l,0}$. Therefore only the first term with $l=0$ is left in (1.194) and contributes to the final

result. So that we need only to calculate $K_0^\dagger(\hat{\Omega})$:

$$K_0^\dagger(\hat{\Omega}) = \int \mathrm{d}\hat{\Omega}_1 \mathrm{d}\hat{\Omega}_L \left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^S (u u_1^* + v v_1^*)^J \cdot (u_1^* v_L^* - v_1^* u_L^*)^{S-J} (u u_L^* + v v_L^*)^J \left(u_L a_L^\dagger + v_L b_L^\dagger\right)^S . \quad (1.201)$$

It is useful to know transformation properties of the integrand in (1.201) under $SU(2)$. The pair of variables (u, v) defined in (1.120) and bosonic annihilation operators (a, b) in the Schwinger representation both transform as spinors under $SU(2)$. That is to say, if we take an arbitrary element $\mathbf{D} \in SU(2)$ (2×2 matrix), then (u, v), *etc.* transform according to

$$\begin{pmatrix} u \\ v \end{pmatrix} \to \mathbf{D} \begin{pmatrix} u \\ v \end{pmatrix} . \quad (1.202)$$

On the other hand, (u^*, v^*), $(-v, u)$, $(a^\dagger, b^\dagger)$ and $(-b, a)$ transform conjugately to (u, v). That is to say (u^*, v^*), *etc.* transform according to

$$\begin{pmatrix} u^* \\ v^* \end{pmatrix} \to \mathbf{D}^* \begin{pmatrix} u^* \\ v^* \end{pmatrix} . \quad (1.203)$$

The combinations appeared in $K_0^\dagger(\hat{\Omega})$ (1.201)

$$u_1 a_1^\dagger + v_1 b_1^\dagger, \quad u u_1^* + v v_1^*, \quad u_1^* v_L^* - v_1^* u_L^*, \quad u u_L^* + v v_L^*, \quad u_L a_L^\dagger + v_L b_L^\dagger \quad (1.204)$$

as well as $A_J^\dagger$ in (1.142), boundary operator $B^\dagger$ in (1.139), *etc.* all transform covariantly under $SU(2)$, *i.e.* those expressions keep their form in the new (transformed) coordinates.

These transformation properties (1.202), (1.203) can be used to simplify the $K_0^\dagger(\hat{\Omega})$ integral. We first make a $SU(2)$ transform

$$\mathbf{D}_{u_L} = \begin{pmatrix} u_L^* & v_L^* \\ -v_L & u_L \end{pmatrix} , \qquad \mathbf{D}_{u_L} \begin{pmatrix} u_L \\ v_L \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad (1.205)$$

under the part of the integral (1.201) over $\hat{\Omega}_1$. Then this part of integral becomes

$$\int \mathrm{d}\hat{\Omega}_1 \left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^S (u u_1^* + v v_1^*)^J (-v_1^*)^{S-J} . \quad (1.206)$$

This can be calculated using binomial expansion and the result is

$$\frac{4\pi}{S+1}\left(ua_1^\dagger + vb_1^\dagger\right)^J\left(-b_1^\dagger\right)^{S-J}. \tag{1.207}$$

Then we make an inverse transform in (1.207) using $\mathbf{D}_{u_L}^{-1} = \mathbf{D}_{u_L}^\dagger$, consequently (1.201) is put in a form with a single integral over $\hat{\Omega}_L$ remaining:

$$\begin{aligned} K_0^\dagger(\hat{\Omega}) &= \frac{4\pi}{S+1}\left(ua_1^\dagger + vb_1^\dagger\right)^J \\ &\cdot \int \mathrm{d}\hat{\Omega}_L \left(a_1^\dagger v_L^* - b_1^\dagger u_L^*\right)^{S-J}\left(uu_L^* + vv_L^*\right)^J\left(u_L a_L^\dagger + v_L b_L^\dagger\right)^S. \end{aligned} \tag{1.208}$$

Now we make another $SU(2)$ transform using

$$\mathbf{D}_u = \begin{pmatrix} u^* & v^* \\ -v & u \end{pmatrix}, \qquad \mathbf{D}_u \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{1.209}$$

then the remaining integral over $\hat{\Omega}_L$ in (1.208) becomes

$$\int \mathrm{d}\hat{\Omega}_L \left(a_1^\dagger v_L^* - b_1^\dagger u_L^*\right)^{S-J}\left(u_L^*\right)^J\left(u_L a_L^\dagger + v_L b_L^\dagger\right)^S. \tag{1.210}$$

Using again binomial expansion, this integral (1.210) yields

$$\frac{4\pi}{S+1}\left(a_1^\dagger b_L^\dagger - b_1^\dagger a_L^\dagger\right)^{S-J}\left(a_L^\dagger\right)^J. \tag{1.211}$$

At last we make an inverse transform in (1.211) using $\mathbf{D}_u^{-1} = \mathbf{D}_u^\dagger$ and plug the result into (1.208), the final form is

$$K_0^\dagger(\hat{\Omega}) = \left(\frac{4\pi}{S+1}\right)^2 A_J^\dagger. \tag{1.212}$$

This expression is consistent with **Conjecture 1.1** (1.196), which also proves that $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ is a set of eigenvectors of the density matrix as $L \to \infty$. Let us denote the density matrix in the limit by $\boldsymbol{\rho}_\infty$. Then (1.212) leads to the result (see (1.198))

$$\boldsymbol{\rho}_\infty|\mathrm{G}; J, \hat{\Omega}\rangle = \frac{1}{(S+1)^2}|\mathrm{G}; J, \hat{\Omega}\rangle. \tag{1.213}$$

We find from (1.213) that the limiting eigenvalue

$$\Lambda_\infty = \frac{1}{(S+1)^2}, \qquad L \to \infty \tag{1.214}$$

is independent of J. Any vector of the $(S+1)^2$-dimensional subspace spanned by the set $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ is an eigenvector of $\boldsymbol{\rho}_\infty$ with the same eigenvalue $\frac{1}{(S+1)^2}$. Therefore $\boldsymbol{\rho}_\infty$ acts on this subspace as (proportional to) the identity $I_{(S+1)^2}$. So that we have proved explicitly that the density matrix takes the form (1.200) in the large block limit. The limiting density matrix is proportional to a projector $\mathbf{P}_{(S+1)^2}$ on the degenerate ground states of the block Hamiltonian H_B (1.141)

$$\boldsymbol{\rho}_\infty = \frac{1}{(S+1)^2}\mathbf{P}_{(S+1)^2}, \qquad L \to \infty. \tag{1.215}$$

In addition, we also derive from the eigenvalues that the von Neumann entropy $S_{\mathrm{v\ N}} = -\sum_{J=0}^{S}(2J+1)\Lambda_\infty \ln \Lambda_\infty$ coincides with the Rényi entropy $S_{\mathrm{R}}(\alpha) = \frac{1}{1-\alpha}\ln\left\{\sum_{J=0}^{S}(2J+1)\Lambda_\infty^\alpha\right\}$ and is equal to the saturated value

$$S_{\mathrm{v\ N}} = S_{\mathrm{R}}(\alpha) = \ln(S+1)^2, \qquad L \to \infty. \tag{1.216}$$

1.5.9 Density Matrix and Correlation Functions

The relation between the density matrix and correlation functions was studied in [4, 31, 32, 50]. It was shown in [31] that the density matrix contains information of all correlation functions in the ground state. The original proof was for spin $S = 1/2$. In this section we generalize the result to generic spin-S as in [50] and the proof is written in a form applicable but not restricted to the AKLT model.

The Hilbert space associated with a spin-S is $(2S+1)$-dimensional. Therefore we could choose a basis of $(2S+1)^2$ linearly independent matrices such that an arbitrary operator defined in the Hilbert space can be written as a superposition over the basis. Let us denote the basis by $\{A_{ab} \mid a, b = 1, \ldots, 2S+1\}$, in which each matrix A_{ab} is labeled by a pair of indices a and b with totally $(2S+1)^2$ possible combinations. The matrix element is defined as

$$(A_{ab})_{kl} = \delta_{ak}\delta_{bl}, \qquad k, l = 1, \ldots, 2S+1. \tag{1.217}$$

In addition to $\{A_{ab}\}$, we introduce an equivalent *conjugate basis* $\{\bar{A}_{ab}\}$ such that

$$(\bar{A}_{ab})_{kl} = \delta_{al}\delta_{bk}, \qquad a, b, k, l = 1, \ldots, 2S+1. \tag{1.218}$$

These matrices (1.217) and (1.218) are actually matrix representation of operators $\{|S,m\rangle\langle S,m'| \mid m,m' = -S,\ldots,S\}$. They are normalized such that

$$\mathrm{tr}(\bar{A}_{ab}A_{cd}) = \sum_{k,l}(\bar{A}_{ab})_{kl}(A_{cd})_{lk} = \sum_{k,l}\delta_{al}\delta_{bk}\delta_{cl}\delta_{dk} = \delta_{ac}\delta_{bd}. \tag{1.219}$$

Here tr takes trace at one and the same site. Because of the completeness of $\{A_{ab}\}$ at each site, the density matrix of the block can be written as (see (1.82))

$$\boldsymbol{\rho}_{\mathrm{block}} = \mathrm{tr}_{\mathrm{outside}}|\mathrm{G}\rangle\langle\mathrm{G}| = \sum_{\{a_jb_j\}}\left(\bigotimes_{j\in\{\mathrm{block}\}}A_{a_jb_j}\right)\mathrm{coeff}\{a_jb_j\}, \tag{1.220}$$

where $|\mathrm{G}\rangle$ denotes the unique ground state, $\mathrm{tr}_{\mathrm{outside}}$ takes traces of sites outside the block and $\mathrm{coeff}\{a_jb_j\}$ denotes the coefficient. Using the normalization property (1.219), the coefficient $\mathrm{coeff}\{a_jb_j\}$ with label j taking values within the block can be expressed as

$$\begin{aligned}
\mathrm{coeff}\{a_jb_j\} &= \sum_{\{c_jd_j\}}\prod_{j\in\mathrm{block}}\mathrm{tr}(\bar{A}_{a_jb_j}A_{c_jd_j})\mathrm{coeff}\{c_jd_j\} \\
&= \mathrm{tr}_{\mathrm{block}}\left[\left(\bigotimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)\boldsymbol{\rho}_{\mathrm{block}}\right] \\
&= \mathrm{tr}_{\mathrm{all}}\left[\left(\bigotimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle\langle\mathrm{G}|\right] \\
&= \langle\mathrm{G}|\left(\bigotimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle.
\end{aligned} \tag{1.221}$$

Here $\mathrm{tr}_{\mathrm{block}}$ takes traces of sites within the block and $\mathrm{tr}_{\mathrm{all}}$ takes traces of all lattice sites. Combing (1.220) with (1.221), we have the final form

$$\boldsymbol{\rho}_{\mathrm{block}} = \sum_{\{a_jb_j\}}\left(\bigotimes_{j\in\{\mathrm{block}\}}A_{a_jb_j}\right)\langle\mathrm{G}|\left(\bigotimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle. \tag{1.222}$$

This is the expression of the density matrix with entries related to multi-point correlation functions $\langle\mathrm{G}|\left(\bigotimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle$ in the ground state. All possible combinations $\{a_jb_j\}$ are involved in the summation. Therefore, we have prove for generic spin-S that the density matrix contains information of

all correlation functions. The matrix elements are all multi-point correlators.

1.6 The 1–dimensional Inhomogeneous Model

The most general 1-dimensional model is the inhomogeneous model in which spins at different lattice site can take different values. As a special case of the generalized model defined in § 1.2.4 , we associate a positive integer number (called multiplicity numbers, see § 1.2.4) to each bond of the lattice and denote by M_{ij} ($M_{ij} = M_{ji}$) the multiplicity number between sites i and j. They are related to bulk spins by the following relation which ensures the existence of a unique ground state

$$2S_j = M_{j-1,j} + M_{j,j+1}, \qquad \forall\ j \tag{1.223}$$

with $2S_0 = M_{01}$ and $2S_{N+1} = M_{N,N+1}$ for ending spins. (Equation (1.223) is a special case of the more general relation (1.23).) The condition for solvability of relation (1.223) is

$$\sum_{j=0}^{N+1}(-1)^j S_j = 0. \tag{1.224}$$

Solution to relation (1.223) under condition (1.224) is

$$M_{j,j+1} = 2\sum_{l=0}^{j}(-1)^{j-l}S_l \geq 1. \tag{1.225}$$

(More details can be found in [36].) Now we defined the Hamiltonian of the inhomogeneous AKLT model according to (1.21) as

$$H = \sum_{j=0}^{N}\ \sum_{J=S_j+S_{j+1}-M_{j,j+1}+1}^{S_j+S_{j+1}} C_J(j,j+1)\pi_J(j,j+1). \tag{1.226}$$

Here the projector $\pi_J(j,j+1)$ describes interactions between neighboring spins j and $j+1$, which projects the bond spin $\boldsymbol{J}_{j,j+1} \equiv \boldsymbol{S}_j + \boldsymbol{S}_{j+1}$ onto the subspace with total spin J ($J = S_j + S_{j+1} - M_{j,j+1} + 1, \ldots, S_j + S_{j+1}$). An explicit expression of $\pi_J(j,j+1)$ is given in § 1.2.2 and [36]. The coefficient $C_J(j,j+1)$ can take an arbitrary positive value. This Hamiltonian (1.226) has a unique ground state (VBS state, see § 1.2.5).

1.6.1 The VBS Ground State

The unique VBS ground state of the Hamiltonian (1.226) is given in the Schwinger representation by [4, 36]

$$|\text{VBS}\rangle \equiv \prod_{j=0}^{N} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^{M_{j,j+1}} |\text{vac}\rangle, \tag{1.227}$$

where $a^\dagger$, $b^\dagger$ are bosonic creation operators defined in exactly the same way as in § 1.2.4 , the constraint on the total boson occupation number is now $\frac{1}{2}(a_j^\dagger a_j + b_j^\dagger b_j) = S_j$. The pure state density matrix of the VBS ground state (1.227) is

$$\boldsymbol{\rho} = \frac{|\text{VBS}\rangle\langle\text{VBS}|}{\langle\text{VBS}|\text{VBS}\rangle}. \tag{1.228}$$

Normalization of the VBS state is (calculation similar to those in § 1.5.1)

$$\langle\text{VBS}|\text{VBS}\rangle = \frac{\prod_{j=0}^{N+1}(2S_j+1)!}{\prod_{j=0}^{N}(M_{j,j+1}+1)}. \tag{1.229}$$

(See [51] for more details.)

1.6.2 The Block Density Matrix

We take a block of L contiguous bulk spins as a subsystem, which starts from site k and ends at site $k+L-1$. Using the coherent state basis (1.121) and completeness relation (1.122), tracing out degrees of freedom outside the block, $\boldsymbol{\rho}_L$ can be written as [32, 51]

$$\boldsymbol{\rho}_L = \tag{1.230}$$
$$\frac{\displaystyle\int \left[\prod_{j=0}^{k-1}\prod_{j=k+L}^{N+1} \mathrm{d}\hat{\Omega}_j\right] \prod_{j=0}^{k-2}\prod_{j=k+L}^{N} \left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^{M_{j,j+1}} B^\dagger|\text{VBS}_L\rangle\langle\text{VBS}_L|B}{\displaystyle\left[\prod_{j=k}^{k+L-1}\frac{(2S_j+1)!}{4\pi}\right]\int\left[\prod_{j=0}^{N+1}\mathrm{d}\hat{\Omega}_j\right]\prod_{j=0}^{N}\left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^{M_{j,j+1}}}.$$

Here the boundary operator B and block VBS state $|\mathrm{VBS}_L\rangle$ are defined as

$$B \equiv \left(u_{k-1}b_k - v_{k-1}a_k\right)^{M_{k-1,k}} \left(a_{k+L-1}v_{k+L} - b_{k+L-1}u_{k+L}\right)^{M_{k+L-1,k+L}}, \tag{1.231}$$

$$|\mathrm{VBS}_L\rangle \equiv \prod_{j=k}^{k+L-2} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^{M_{j,j+1}} |\mathrm{vac}\rangle, \tag{1.232}$$

respectively. After performing integrals over $\hat{\Omega}_j$ $(j = 0, 1, \ldots, k-2, k+L+1, \ldots, N, N+1)$ in the numerator and all integrals in the denominator, the density matrix $\boldsymbol{\rho}_L$ turns out to be independent of spins outside the block. This property has been proved for the homogeneous AKLT model in § 1.5.2 (see also [11, 32, 50]). Therefore, we can re-label spins within the block for notational convenience. Let $k = 1$ and the density matrix takes the form

$$\boldsymbol{\rho}_L = \frac{\prod_{j=0}^{L}(M_{j,j+1}+1)}{\prod_{j=1}^{L}(2S_j+1)!} \frac{1}{(4\pi)^2} \int \mathrm{d}\hat{\Omega}_0 \mathrm{d}\hat{\Omega}_{L+1} B^\dagger |\mathrm{VBS}_L\rangle\langle\mathrm{VBS}_L| B \tag{1.233}$$

with

$$B^\dagger = \left(u_0^* b_1^\dagger - v_0^* a_1^\dagger\right)^{M_{0,1}} \left(a_L^\dagger v_{L+1}^* - b_L^\dagger u_{L+1}^*\right)^{M_{L,L+1}}, \tag{1.234}$$

$$|\mathrm{VBS}_L\rangle = \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^{M_{j,j+1}} |\mathrm{vac}\rangle. \tag{1.235}$$

Again, the remaining two integrals in (1.233) are kept in the present form for later use.

1.6.3 Ground States of the Block Hamiltonian

The block Hamiltonian with the re-labeling $k = 1$ reads

$$H_B = \sum_{j=1}^{L-1} \sum_{J=S_j+S_{j+1}-M_{j,j+1}+1}^{S_j+S_{j+1}} C_J(j, j+1) P_J(j, j+1). \tag{1.236}$$

Now the degenerate ground states are constructed in a similar way as in § 1.5.3 . The new $A_J^\dagger$ operator is defined as:

$$A_J^\dagger \equiv \left(ua_1^\dagger + vb_1^\dagger\right)^{J_-+J} \left(a_1^\dagger b_L^\dagger - b_1^\dagger a_L^\dagger\right)^{J_+-J} \left(ua_L^\dagger + vb_L^\dagger\right)^{-J_-+J}, \quad (1.237)$$

where $J_- \equiv \frac{1}{2}(M_{01} - M_{L,L+1})$, $J_+ \equiv \frac{1}{2}(M_{01} + M_{L,L+1})$ and $|J_-| \leq J \leq J_+$. Then the set of ground states of the block Hamiltonian (1.236) is

$$|\mathrm{G}; J, \hat{\Omega}\rangle \equiv A_J^\dagger |\mathrm{VBS}_L\rangle, \qquad J = |J_-|, \ldots, J_+. \quad (1.238)$$

To prove that any state $|\mathrm{G}; J, \hat{\Omega}\rangle$ is a zero-energy ground state of (1.236), we essentially repeat the arguments as in § 1.5.3 for any site j and bond $(j, j+1)$:

1. The total power of $a_j^\dagger$ and $b_j^\dagger$ is $2S_j$, so that we have spin-S_j at site j;
2. $-\frac{1}{2}(M_{j-1,j} + M_{j+1,j+2}) \leq J_{j,j+1}^z \equiv S_j^z + S_{j+1}^z \leq \frac{1}{2}(M_{j-1,j} + M_{j+1,j+2})$ by a binomial expansion, so that the maximum value of the bond spin $J_{j,j+1}$ is $\frac{1}{2}(M_{j-1,j} + M_{j+1,j+2}) = S_j + S_{j+1} - M_{j,j+1}$ (from $SU(2)$ invariance, see [4]).

Therefore, the state $|\mathrm{G}; J, \hat{\Omega}\rangle$ defined in (1.238) has spin-S_j at site j and no projection onto the $J_{j,j+1} > S_j + S_{j+1} - M_{j,j+1}$ subspace for any bond.

Parallelly, we also introduce an orthogonal basis in description of the degenerate zero-energy ground states of H_B (1.236), *i.e.* the degenerate VBS states. Using the same notations as in § 1.5.3 , the operator $A_J^\dagger$ defined in (1.237) can be expanded as (see [25, 51])

$$\begin{aligned} A_J^\dagger \;=\; & \sqrt{\frac{(J_+ + J + 1)!(J_- + J)!(J_+ - J)!(-J_- + J)!}{2J+1}} \sum_{M=-J}^{J} X_{JM} \quad (1.239) \\ & \cdot \sum_{m_1, m_L}^{m_1+m_L=M} (\frac{1}{2}M_{01}, m_1; \frac{1}{2}M_{L,L+1}, m_L | J, M)\; \psi^\dagger_{\frac{1}{2}M_{01}, m_1} \otimes \psi^\dagger_{\frac{1}{2}M_{L,L+1}, m_L}, \end{aligned}$$

where $(\frac{1}{2}M_{01}, m_1; \frac{1}{2}M_{L,L+1}, m_L | J, M)$ is the Clebsch-Gordan coefficient. Again, the particular form of the sum over m_1 and m_L in (1.239) is identified as a single spin state creation operator

$$\Psi^\dagger_{JM} \equiv \sum_{m_1, m_L}^{m_1+m_L=M} (\frac{1}{2}M_{01}, m_1; \frac{1}{2}M_{L,L+1}, m_L | J, M)\; \psi^\dagger_{\frac{1}{2}M_{01}, m_1} \otimes \psi^\dagger_{\frac{1}{2}M_{L,L+1}, m_L}. \quad (1.240)$$

So that the set of *degenerate VBS states* $\{|\mathrm{VBS}_L(J,M)\rangle\}$ is defined as

$$|\mathrm{VBS}_L(J,M)\rangle \equiv \Psi^\dagger_{JM}|\mathrm{VBS}_L\rangle, \quad J=|J_-|,...,J_+, \quad M=-J,...,J. \tag{1.241}$$

Then these $(M_{01}+1)(M_{L,L+1}+1)$ states (1.241) are mutually orthogonal (the proof is exactly the same as in § 1.5.3). Also, the state $|\mathrm{G};J,\hat{\Omega}\rangle$ written as a linear superposition over these degenerate VBS states reads

$$\begin{aligned} |\mathrm{G};J,\hat{\Omega}\rangle &= \sqrt{\frac{(J_++J+1)!(J_-+J)!(J_+-J)!(-J_-+J)}{2J+1}} \\ &\quad \cdot \sum_{M=-J}^{J} X_{JM}|\mathrm{VBS}_L(J,M)\rangle. \end{aligned} \tag{1.242}$$

Therefore, as seen from (1.242), the rank of set of states $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ with the same J value is $2J+1$ and the total number of linearly independent states of the set $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ is $\sum_{J=|J_-|}^{J_+}(2J+1)=(M_{01}+1)(M_{L,L+1}+1)$, which is exactly the degeneracy of the ground states of (1.236). So that $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ forms a complete set of zero-energy ground states. The orthogonal set $\{|\mathrm{VBS}_L(J,M)\rangle\}$ also forms a complete set of zero-energy ground states, which differs from $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ by a change of basis.

1.6.4 Diagonalization of the Density Matrix

The density matrix is diagonalized in § 1.5.4 and § 1.5.5 for the homogeneous AKLT model. The analysis can be made in parallel for the inhomogeneous model.

The statement of **Theorem 1.2** is still valid here. *i.e.* Eigenvectors of the density matrix $\boldsymbol{\rho}_L$ (1.233) with non-zero eigenvalues are given by the set $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ (1.238) or $\{|\mathrm{VBS}_L(J,M)\rangle\}$ (1.241). This explicit construction of eigenvectors yields a direct diagonalization of the density matrix.

Again, we prove the theorem by re-writing the density matrix $\boldsymbol{\rho}_L$ (1.233) as a projector in diagonal form onto the orthogonal degenerate VBS states $\{|\mathrm{VBS}_L(J,M)\rangle\}$ introduced in (1.241).

Take expression (1.233) and integrate over $\hat{\Omega}_0$ and $\hat{\Omega}_{L+1}$ using binomial

expansions and $\int_{-1}^{1} \mathrm{d}x(1+x)^m(1-x)^n = \frac{m!n!}{(m+n+1)!}2^{m+n+1}$. Then we have

$$\begin{aligned}
\boldsymbol{\rho}_L &= \frac{\prod_{j=1}^{L-1}(M_{j,j+1}+1)}{\prod_{j=1}^{L}(2S_j+1)!}\sum_{p=0}^{M_{01}}\sum_{q=0}^{M_{L,L+1}}\begin{pmatrix} M_{01} \\ p \end{pmatrix}\begin{pmatrix} M_{L,L+1} \\ q \end{pmatrix} \\
&\quad (b_1^\dagger)^p(a_1^\dagger)^{M_{01}-p}(a_L^\dagger)^q(b_L^\dagger)^{M_{L,L+1}-q}|\mathrm{VBS}_L\rangle \\
&\quad \langle\mathrm{VBS}_L|(b_L)^{M_{L,L+1}-q}(a_L)^q(a_1)^{M_{01}-p}(b_1)^p. \qquad (1.243)
\end{aligned}$$

The particular combinations of bosonic operators appeared in (1.243) are recognized up to a constant as spin creation operators $\psi^\dagger_{\frac{1}{2}M_{01},\frac{1}{2}M_{01}-p}$ and $\psi^\dagger_{\frac{1}{2}M_{L,L+1},q-\frac{1}{2}M_{L,L+1}}$ at site 1 and site L, respectively. They commute with all bond operators $\left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^{M_{j,j+1}}$, so that we could simplify the right hand side of (1.243) using definition (1.240) and the following identity:

$$\begin{aligned}
&\sum_{p=0}^{M_{01}}\sum_{q=0}^{M_{L,L+1}} \psi^\dagger_{\frac{1}{2}M_{01},\frac{1}{2}M_{01}-p}\otimes\psi^\dagger_{\frac{1}{2}M_{L,L+1},q-\frac{1}{2}M_{L,L+1}}|\mathrm{vac}\rangle_{1,L} \\
&{}_{1,L}\langle\mathrm{vac}|\psi_{\frac{1}{2}M_{01},\frac{1}{2}M_{01}-p}\otimes\psi_{\frac{1}{2}M_{L,L+1},q-\frac{1}{2}M_{L,L+1}} \\
=\ &\sum_{p=0}^{M_{01}}\sum_{q=0}^{M_{L,L+1}} |\frac{1}{2}M_{01},\frac{1}{2}M_{01}-p\rangle_1\langle\frac{1}{2}M_{01},\frac{1}{2}M_{01}-p| \\
&\otimes|\frac{1}{2}M_{L,L+1},q-\frac{1}{2}M_{L,L+1}\rangle_L\langle\frac{1}{2}M_{L,L+1},q-\frac{1}{2}M_{L,L+1}| \\
=\ &\sum_{J=|J_-|}^{J_+}\sum_{M=-J}^{J}|J,M\rangle_{1,L}\langle J,M| \\
=\ &\sum_{J=|J_-|}^{J_+}\sum_{M=-J}^{J}\Psi^\dagger_{JM}|\mathrm{vac}\rangle_{1,L}\langle\mathrm{vac}|\Psi_{JM}. \qquad (1.244)
\end{aligned}$$

The resultant final form of density matrix $\boldsymbol{\rho}_L$ is then

$$\begin{aligned}\boldsymbol{\rho}_L &= \frac{\prod_{j=1}^{L-1}(M_{j,j+1}+1)}{\prod_{j=1}^{L}(2S_j+1)!}M_{01}!M_{L,L+1}!\sum_{J=|J_-|}^{J_+}\sum_{M=-J}^{J}\Psi^\dagger_{JM}|\mathrm{VBS}_L\rangle\langle\mathrm{VBS}_L|\Psi_{JM}\\ &= \frac{\prod_{j=1}^{L-1}(M_{j,j+1}+1)}{\prod_{j=1}^{L}(2S_j+1)!}M_{01}!M_{L,L+1}!\sum_{J=|J_-|}^{J_+}\sum_{M=-J}^{J}|\mathrm{VBS}_L(J,M)\rangle\langle\mathrm{VBS}_L(J,M)|.\end{aligned} \tag{1.245}$$

The set of degenerate VBS states $\{|\mathrm{VBS}_L(J,M)\rangle\}$ with $J=|J_-|,\ldots,J_+$ and $M=-J,\ldots,J$ forms an orthogonal basis. These $(M_{01}+1)(M_{L,L+1}+1)$ states also forms a complete set of zero-energy ground states of the block Hamiltonian (1.236). So that in expression (1.245) we have re-written the density matrix as a projector in diagonal form over an orthogonal basis. Each degenerate VBS state $|\mathrm{VBS}_L(J,M)\rangle$ is an eigenvector of the density matrix, so as any of the state $|\mathrm{G};J,\hat{\Omega}\rangle$ (because of the degeneracy of corresponding eigenvalues of the density matrix, see § 1.6.5). Thus we have generalized **Theorem 1.2** to the inhomogeneous case.

1.6.5 Eigenvalues of the Density Matrix

Given the diagonalized form (1.245), again eigenvalues of the density matrix $\boldsymbol{\rho}_L$ are derived from normalization of degenerate VBS states with an explicit expression in terms of Wigner $3j$-symbols.

Similarly, we first calculate the integral of the norm square of $|\mathrm{G};J,\hat{\Omega}\rangle$over the unit vector $\hat{\Omega}$

$$\begin{aligned}&\frac{1}{4\pi}\int \mathrm{d}\hat{\Omega}\langle\mathrm{G};J,\hat{\Omega}|\mathrm{G};J,\hat{\Omega}\rangle \\ =\ &\frac{(J_++J+1)!(J_-+J)!(J_+-J)!(-J_-+J)!}{(2J+1)!}\langle\mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle.\end{aligned} \tag{1.246}$$

This expression (1.246) also states that normalization of the degenerate VBS state is independent of $\hat{\Omega}$ and/or M.

Let us consider the integral involved in (1.246). Using coherent state basis

(1.121) and completeness relation (1.122) as before, we obtain

$$\begin{aligned} & \frac{1}{4\pi}\int \mathrm{d}\hat{\Omega}\langle \mathrm{G}; J, \hat{\Omega}|\mathrm{G}; J, \hat{\Omega}\rangle \qquad (1.247)\\ = \; & \frac{1}{4\pi}\left[\prod_{j=1}^{L}\frac{(2S_j+1)!}{4\pi}\right]\int \mathrm{d}\hat{\Omega}\int\left[\prod_{j=1}^{L}\mathrm{d}\hat{\Omega}_j\right]\prod_{j=1}^{L-1}\left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^{M_{j,j+1}} \\ \cdot \; & \left[\frac{1}{2}(1-\hat{\Omega}_1\cdot\hat{\Omega}_L)\right]^{J_+-J}\left[\frac{1}{2}(1+\hat{\Omega}_1\cdot\hat{\Omega})\right]^{J_-+J}\left[\frac{1}{2}(1+\hat{\Omega}\cdot\hat{\Omega}_L)\right]^{-J_-+J}. \end{aligned}$$

Now we expand $\left[\frac{1}{2}(1-\hat{\Omega}_i\cdot\hat{\Omega}_j)\right]^{M_{ij}}$ in terms of spherical harmonics

$$\left[\frac{1}{2}(1-\hat{\Omega}_i\cdot\hat{\Omega}_j)\right]^{M_{ij}} = \frac{4\pi}{M_{ij}+1}\sum_{l=0}^{M_{ij}}\lambda(l,M_{ij})\sum_{m=-l}^{l}Y_{lm}(\hat{\Omega}_i)Y^*_{lm}(\hat{\Omega}_j) \qquad (1.248)$$

with

$$\lambda(l,M_{ij}) = \frac{(-1)^l M_{ij}!(M_{ij}+1)!}{(M_{ij}-l)!(M_{ij}+l+1)!}. \qquad (1.249)$$

Then integrate over $\hat{\Omega}$ and from $\hat{\Omega}_2$ to $\hat{\Omega}_{L-1}$, the right hand side of (1.247) is equal to

$$\begin{aligned} & \frac{4\pi\prod_{j=1}^{L}(2S_j+1)!}{\left[\prod_{j=1}^{L-1}(M_{j,j+1}+1)\right](J_-+J+1)(J_+-J+1)(-J_-+J+1)} \\ \cdot \; & \sum_{l}^{M_<}\sum_{l_\alpha=0}^{J_+-J}\sum_{l_\beta=0}^{J_<}\sum_{m=-l}^{l}\sum_{m_\alpha=-l_\alpha}^{l_\alpha}\sum_{m_\beta=-l_\beta}^{l_\beta}\left[\prod_{j=1}^{L-1}\lambda(l,M_{j,j+1})\right] \\ \cdot \; & \lambda(l_\alpha,J_+-J)\lambda(l_\beta,J_-+J)\lambda(l_\beta,-J_-+J)\int \mathrm{d}\hat{\Omega}_1\int \mathrm{d}\hat{\Omega}_L \\ \cdot \; & Y_{l,m}(\hat{\Omega}_1)Y_{l_\alpha,m_\alpha}(\hat{\Omega}_1)Y_{l_\beta,m_\beta}(\hat{\Omega}_1)Y^*_{l,m}(\hat{\Omega}_L)Y^*_{l_\alpha,m_\alpha}(\hat{\Omega}_L)Y^*_{l_\beta,m_\beta}(\hat{\Omega}_L). \end{aligned} \qquad (1.250)$$

Where we have $M_< \equiv \min\{M_{j,j+1}, j = 1,\ldots,L-1\}$ and $J_< \equiv \min\{J_-+J, -J_-+J\}$, both being the minimum of the corresponding set. Now we carry

out remaining integrals in (1.250) using

$$\begin{aligned}&\int \mathrm{d}\hat{\Omega} Y_{l,m}(\hat{\Omega}) Y_{l_\alpha,m_\alpha}(\hat{\Omega}) Y_{l_\beta,m_\beta}(\hat{\Omega}) \\ &= \sqrt{\frac{(2l+1)(2l_\alpha+1)(2l_\beta+1)}{4\pi}} \begin{pmatrix} l & l_\alpha & l_\beta \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l_\alpha & l_\beta \\ m & m_\alpha & m_\beta \end{pmatrix}.\end{aligned} \tag{1.251}$$

The result after integration can be further simplified by applying the following orthogonality relation

$$\sum_{m,m_\alpha} (2l_\beta+1) \begin{pmatrix} l & l_\alpha & l_\beta \\ m & m_\alpha & m_\beta \end{pmatrix} \begin{pmatrix} l & l_\alpha & l'_\beta \\ m & m_\alpha & m'_\beta \end{pmatrix} = \delta_{l_\beta l'_\beta} \delta_{m_\beta m'_\beta}, \tag{1.252}$$

where $\begin{pmatrix} l & l_\alpha & l_\beta \\ m & m_\alpha & m_\beta \end{pmatrix}$, *etc.* are the Wigner $3j$-symbols.

So that finally expression (1.250) is equal to

$$\begin{aligned}&\frac{\prod_{j=1}^{L}(2S_j+1)!}{\left[\prod_{j=1}^{L-1}(M_{j,j+1}+1)\right](J_-+J+1)(J_+-J+1)(-J_-+J+1)} \\ &\cdot \sum_{l}^{M_<} \sum_{l_\alpha=0}^{J_+-J} \sum_{l_\beta=0}^{J_<} \left[\prod_{j=1}^{L-1} \lambda(l, M_{j,j+1})\right] \lambda(l_\alpha, J_+-J) \lambda(l_\beta, J_-+J) \lambda(l_\beta, -J_-+J) \\ &\cdot (2l+1)(2l_\alpha+1)(2l_\beta+1) \begin{pmatrix} l & l_\alpha & l_\beta \\ 0 & 0 & 0 \end{pmatrix}^2.\end{aligned} \tag{1.253}$$

The explicit value of $\begin{pmatrix} l & l_\alpha & l_\beta \\ 0 & 0 & 0 \end{pmatrix}$ is given by

$$\begin{aligned}&\begin{pmatrix} l & l_\alpha & l_\beta \\ 0 & 0 & 0 \end{pmatrix} \\ &= (-1)^g \sqrt{\frac{(2g-2l)!(2g-2l_\alpha)!(2g-2l_\beta)!}{(2g+1)!}} \frac{g!}{(g-l)!(g-l_\alpha)!(g-l_\beta)!},\end{aligned} \tag{1.254}$$

if $l+l_\alpha+l_\beta = 2g$ ($g \in \mathbf{N}$), otherwise zero.

Combining results of (1.245), (1.246) and (1.253), we arrive at the following

result for eigenvalues: Eigenvalues $\Lambda(J)$ ($J = |J_-|, \ldots, J_+$) of the density matrix are independent of $\hat{\Omega}$ and/or M in defining eigenvectors (see (1.238) and (1.241)). An explicit expression is given by the following triple sum

$$\begin{aligned}\Lambda(J) &= \frac{\prod_{j=1}^{L-1}(M_{j,j+1}+1)}{\prod_{j=1}^{L}(2S_j+1)!} M_{01}!M_{L,L+1}!\langle \mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle \qquad (1.255)\\ &= \frac{(2J+1)!M_{01}!M_{L,L+1}!}{(J_++J+1)!(J_-+J+1)!(J_+-J+1)!(-J_-+J+1)!}\\ &\cdot \sum_{l}^{M_<}\sum_{l_\alpha=0}^{J_+-J}\sum_{l_\beta=0}^{J_<}\left[\prod_{j=1}^{L-1}\lambda(l,M_{j,j+1})\right]\lambda(l_\alpha,J_+-J)\lambda(l_\beta,J_-+J)\lambda(l_\beta,-J_-+J)\\ &\cdot (2l+1)(2l_\alpha+1)(2l_\beta+1)\begin{pmatrix} l & l_\alpha & l_\beta\\ 0 & 0 & 0\end{pmatrix}^2.\end{aligned}$$

1.6.6 The Large Block Limit

In this section, we generalize the characteristic properties (§ 1.5.8) of the limiting density matrix to the inhomogeneous model.

Let us apply the density matrix $\boldsymbol{\rho}_L$ (1.233) to the state $|\mathrm{G};J,\hat{\Omega}\rangle$ (1.238) and get

$$\begin{aligned}&\boldsymbol{\rho}_L|\mathrm{G};J,\hat{\Omega}\rangle \qquad (1.256)\\ &= \frac{\prod_{j=0}^{L}(M_{j,j+1}+1)}{\prod_{j=1}^{L}(2S_j+1)!}\frac{1}{(4\pi)^2}\int \mathrm{d}\hat{\Omega}_0\mathrm{d}\hat{\Omega}_{L+1}B^\dagger|\mathrm{VBS}_L\rangle\langle\mathrm{VBS}_L|BA_J^\dagger|\mathrm{VBS}_L\rangle.\end{aligned}$$

Using the coherent state basis (1.121) and completeness relation (1.122), the

factor $\langle \mathrm{VBS}_L | B A_J^\dagger | \mathrm{VBS}_L \rangle$ in (1.190) can be re-written as

$$\begin{aligned} & \langle \mathrm{VBS}_L | B A_J^\dagger | \mathrm{VBS}_L \rangle \\ = & \left[\prod_{j=1}^{L} \frac{(2S_j+1)!}{4\pi} \right] \int \left(\prod_{j=1}^{L} \mathrm{d}\hat{\Omega}_j \right) \prod_{j=1}^{L-1} \left[\frac{1}{2}(1 - \hat{\Omega}_j \cdot \hat{\Omega}_{j+1}) \right]^{M_{j,j+1}} \\ & \cdot (u_0 v_1 - v_0 u_1)^{M_{01}} \left(u u_1^* + v v_1^* \right)^{J_- + J} \left(u_1^* v_L^* - v_1^* u_L^* \right)^{J_+ - J} \\ & \cdot \left(u u_L^* + v v_L^* \right)^{-J_- + J} \left(u_L v_{L+1} - v_L u_{L+1} \right)^{M_{L,L+1}} . \end{aligned} \tag{1.257}$$

We plug the expression (1.257) into (1.256). Using transformation properties under $SU(2)$ and a binomial expansion, the integral over $\hat{\Omega}_0$ yields that

$$\int \mathrm{d}\hat{\Omega}_0 \left(u_0^* b_1^\dagger - v_0^* a_1^\dagger \right)^{M_{01}} (u_0 v_1 - v_0 u_1)^{M_{01}} = \frac{4\pi}{M_{01}+1} \left(u_1 a_1^\dagger + v_1 b_1^\dagger \right)^{M_{01}} . \tag{1.258}$$

Similarly we can perform the integral over $\hat{\Omega}_{L+1}$. Then using expansion (1.248) and orthogonality of spherical harmonics, other integrals over $\hat{\Omega}_j$ with $j = 2, \ldots, L-1$ in (1.257) can be performed. As a result, the following expression is obtained from (1.256):

$$\boldsymbol{\rho}_L | \mathrm{G}; J, \hat{\Omega} \rangle = \frac{1}{(4\pi)^2} \sum_{l=0}^{M_<} (2l+1) \left[\prod_{j=1}^{L-1} \lambda(l, M_{j,j+1}) \right] K_l^\dagger(\hat{\Omega}) \, | \mathrm{VBS}_L \rangle . \tag{1.259}$$

The operator $K_l^\dagger(\hat{\Omega})$ involved in (1.259) is defined as

$$\begin{aligned} K_l^\dagger(\hat{\Omega}) \equiv & \int \mathrm{d}\hat{\Omega}_1 \mathrm{d}\hat{\Omega}_L P_l(\hat{\Omega}_1 \cdot \hat{\Omega}_L) \left(u_1 a_1^\dagger + v_1 b_1^\dagger \right)^{M_{01}} \left(u u_1^* + v v_1^* \right)^{J_- + J} \\ & \cdot \left(u_1^* v_L^* - v_1^* u_L^* \right)^{J_+ - J} \left(u u_L^* + v v_L^* \right)^{-J_- + J} \left(u_L a_L^\dagger + v_L b_L^\dagger \right)^{M_{L,L+1}} . \end{aligned} \tag{1.260}$$

It is expressed as an integral depending on the order l of the Legendre polynomial $P_l(\hat{\Omega}_1 \cdot \hat{\Omega}_L)$.

There was no ambiguity in defining the large block limit in the homogeneous AKLT model (see § 1.5.8). However, in the inhomogeneous model we must specify the behavior of ending spins in the large block limit. So we define the large block limit as when $L \to \infty$, the two ending spins approach definite values, namely, $M_{01} \to S_-$ and $M_{L,L+1} \to S_+$. Then we realize from (1.249) that as $L \to \infty$, $\prod_{j=1}^{L-1} \lambda(l, M_{j,j+1}) \to \delta_{l,0}$. Therefore only the first term with

$l = 0$ is left in (1.259). So that we need only to calculate the limiting $K_0^\dagger(\hat{\Omega})$:

$$K_0^\dagger(\hat{\Omega}) \overset{L\to\infty}{\longrightarrow} \int \mathrm{d}\hat{\Omega}_1 \mathrm{d}\hat{\Omega}_L \left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^{S_-} (uu_1^* + vv_1^*)^{J_- + J} \cdot (u_1^* v_L^* - v_1^* u_L^*)^{J_+ - J} (uu_L^* + vv_L^*)^{-J_- + J} \left(u_L a_L^\dagger + v_L b_L^\dagger\right)^{S_+}. \tag{1.261}$$

Here both J_- and J_+ take the limiting values $\frac{1}{2}(S_- - S_+)$ and $\frac{1}{2}(S_- + S_+)$, respectively.

Using transformation properties of the integrand in (1.261) under $SU(2)$, the $K_0^\dagger(\hat{\Omega})$ integral is simplified and carried out as

$$K_0^\dagger(\hat{\Omega}) = \frac{(4\pi)^2}{(S_- + 1)(S_+ + 1)} A_J^\dagger. \tag{1.262}$$

This expression states that $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ is a set of eigenvectors of the density matrix as $L \to \infty$. Let us denote the density matrix in the limit by $\boldsymbol{\rho}_\infty$. Then (1.262) leads to the result (see (1.259))

$$\boldsymbol{\rho}_\infty |\mathrm{G}; J, \hat{\Omega}\rangle = \frac{1}{(S_- + 1)(S_+ + 1)} |\mathrm{G}; J, \hat{\Omega}\rangle. \tag{1.263}$$

We find from (1.263) that the limiting eigenvalue

$$\Lambda_\infty = \frac{1}{(S_- + 1)(S_+ + 1)}, \qquad L \to \infty \tag{1.264}$$

is independent of J. Any vector of the $(S_- + 1)(S_+ + 1)$-dimensional subspace spanned by the set $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ is an eigenvector of $\boldsymbol{\rho}_\infty$ with the same eigenvalue $\frac{1}{(S_- + 1)(S_+ + 1)}$. Therefore $\boldsymbol{\rho}_\infty$ is proportional to a projector $\mathbf{P}_{(S_- + 1)(S_+ + 1)}$:

$$\boldsymbol{\rho}_\infty = \frac{1}{(S_- + 1)(S_+ + 1)} \mathbf{P}_{(S_- + 1)(S_+ + 1)}, \tag{1.265}$$

which is a generalization of (1.215) to the inhomogeneous model. In addition, we also derive from the eigenvalues that the von Neumann entropy $S_{\mathrm{v\ N}}$ coincides with the Renyi entropy S_{R} and is equal to the saturated value $\ln[(S_- + 1)(S_+ + 1)]$.

1.7 Summary

We have studied the entanglement of the VBS ground state for the AKLT model in this chapter. The AKLT model is formulated on an arbitrary connected graph or a lattice. The Hamiltonian (1.14), (1.21) is a sum of projectors which describe interactions between nearest neighbors. The condition of uniqueness of the ground state relates the spin value at each vertex (site) with multiplicity numbers associated with edges incident to the vertex (bonds connected to the site), see (1.15), (1.23), (1.24). The unique ground state is known as the Valence-Bond-Solid state (1.20), (1.31).

To study the entanglement, the graph (lattice) is divided into two parts: the *block* and the *environment*. We investigate the density matrix $\boldsymbol{\rho}_B$ of the block and show that it has many zero eigenvalues. We describe the subspace (called the *support*) of eigenvectors of $\boldsymbol{\rho}_B$ with non-zero eigenvalues. It has been proved (see **Theorem 1.1** in § 1.3.3) that this subspace is the degenerate *ground space* of some Hamiltonian which is called the *block* Hamiltonian H_B (1.58).

The entanglement can be measured by the von Neumann entropy or the Rényi entropy of the density matrix $\boldsymbol{\rho}_B$. Most eigenvalues of $\boldsymbol{\rho}_B$ vanish and have no contribution to the entanglement entropies. The density matrix takes the form of a projector on the *ground space* of H_B multiplied by another matrix (see also [52]).

A complete analysis of the density matrix for a variety of 1-dimensional AKLT models has been presented. The block density matrix $\boldsymbol{\rho}_L$ for a subsystem of L contiguous bulk spins has been diagonalized with non-zero eigenvalues calculated (see also [11, 32, 50, 51]). We find that in all these cases the *support* coincide with the *ground space*, so their dimensions are equal $D = deg$. In the large block limit, all non-zero eigenvalues become the same and the density matrix is proportional to a projector (1.215), (1.265). The von Neumann entropy equals the Rényi entropy and both take the saturated value $S_{\text{v N}} = S_{\text{R}} = \ln D = \ln(deg)$.

Moreover, it turns out that the block Hamiltonian H_B defines the density matrix $\boldsymbol{\rho}_L$ completely in the large block limit $L \to \infty$. The zero-energy ground states of the block Hamiltonian H_B span the subspace that the density matrix $\boldsymbol{\rho}_L$ projects onto. So that $\boldsymbol{\rho}_L$ can be represented as the zero-temperature limit of the canonical ensemble density matrix defined by H_B:

$$\boldsymbol{\rho}_L = \lim_{\beta \to +\infty} \frac{\mathrm{e}^{-\beta H_B}}{\mathrm{tr}\,[\ \mathrm{e}^{-\beta H_B}\ ]}, \qquad L \to \infty. \tag{1.266}$$

In the zero-temperature limit, contributions from excited states of H_B all

vanish and the right hand side of (1.266) turns into a projector onto the ground states of the block Hamiltonian.

For more complicated graphs or lattices, non-zero eigenvalues of the density matrix are still unknown. One open problem is to calculate those eigenvalues. One may start with the Cayley tree (also known as the Bethe tree) and an exact explicit expression for the non-zero eigenvalues is expected because there is no loop. It is also important to calculate non-zero eigenvalues of $\boldsymbol{\rho}_B$ for graphs with loops. In all known examples [11, 50, 51] where the density matrix of a large block has been calculated, all non-zero eigenvalues coincide. So that the density matrix of a large block is proportional to a projector. We *conjecture* that this will be the case for all connected graphs. In other words, we expect that in the large block limit, each non-zero eigenvalue should approach the same value $\frac{1}{D} = \frac{1}{deg}$, thus the entanglement entropies should be saturated, *i.e.* $S_{\text{v N}} = S_{\text{R}} = \ln D = \ln(deg)$. The density matrix should be proportional to a projector on the ground space of the block Hamiltonian, *i.e.* $\boldsymbol{\rho}_B = \frac{1}{D}\mathbf{P}_D = \frac{1}{deg}\mathbf{P}_{deg}$.

Chapter 2

Quantum Search Algorithms

2.1 Introduction

One spectacular promise of a quantum computer is to enable new algorithms which could practically solve feasible problems requiring exorbitant resources on a classical computer. Two broad classes of quantum algorithms are known which fulfill this promise. The first class is based on the Shor's quantum Fourier transform, which includes algorithms for solving the factorization problem with a exponential speedup over corresponding classical algorithms. The second class is based on Grover's algorithm for performing quantum database searching which provides a quadratic speedup over the classical algorithms. This chapter is devoted to the subject of quantum search.

Database search has many applications and it appears in everyday life. Search algorithm enters as a subroutine in many important algorithms in computer sciences [41, 54, 55]. L. Grover discovered a quantum algorithm [56] which searches an *unsorted* database faster than any classical algorithm in 1996. By *unsorted* we mean that there is no arrangement of items in some sequence or particular order for searching. for example, a phonebook with names listed alphabetically is a sorted database when we are looking for the phone number associated with a given name; however, the same phone book becomes an unsorted database if we are provided with a phone number and looking for the name. Suppose that we have a large database of N items and we are searching for one item, called the *target item* or *solution*. (*e.g.* Given a map containing many cities, wishing to determine the shortest route passing through all cities on the map.) Technically, rather than search the elements directly, we concentrate on the *index* or *address* of those items, which is just a number in the range 0 to $N-1$. For convenience assuming $N = 2^n$ (it is always possible to add additional auxiliary items to make the number N a

power of 2), so the address can be stored in n bits. Let us denote the addresses of items by x and that of the target by t. (Without confusion, we could identify the address with the actual item. For the quantum case, each address data x is associated with a vector $|x\rangle$ which contains n qubits and the database is a N-dimensional Hilbert space.) For an unsorted database, we are only provided with a testing function $f(x)$, which takes as input an arbitrary x from the database. By definition, the output of f is 1 if x is a solution to the search problem, and 0 if not. In other words, f is a black box with the ability to recognize the solution to the search problem. The internal workings of f are not important in our discussion, but the value is that $f(x) = \delta_{x,t}$. This test function is called an *oracle*. (It has a quantum version which is discussed in § 2.2.1 .) We use number of queries to the oracle as complexity measure. Any classical algorithm (essentially a random picking up of items) takes $\mathcal{O}(N)$ number of queries. The Grover algorithm finds the target item (with probability 1) in

$$j_{\text{full}} = \frac{\pi}{4}\sqrt{N} \sim \mathcal{O}\left(\sqrt{N}\right), \qquad N \to \infty \tag{2.1}$$

iterations (queries to the oracle), which is a quadratic speedup. We shall call it a *full search*.

It occurs frequently in practice that less information is needed. For example, the address of the target item in binary form is $|t\rangle = |b_1 b_2 b_3 ... b_n\rangle$, and we want to find only the first 3 bits $b_1 b_2 b_3$. This means that the database is partitioned into 8 blocks. All items in a block share the common feature such that the first 3 bits being the same. We want to find the block containing the target item. This is an example of partial search. The general problem of partial search considers the following: An N item database is partitioned into K blocks, each of the same size

$$b = \frac{N}{K}. \tag{2.2}$$

A user wants to find the block containing the target item, instead of the target item itself. The block with the target item is called the *target block*; others non-target blocks. Partial search naturally arises in list matching [58]. Partial search is not only a compromise on accuracy for speed, but also has it own significance. Partial search can find all items in the database which share some features with the target item. This can be considered as a special case of sorting problem. The GRK algorithm of partial search was suggested by Grover and Radhakrishnan [57] and optimized in [59]. It takes $\sim \frac{\pi}{4}(1 - \text{coeff}(K))\sqrt{N}$ number of queries to find the target block. Here coeff(K) is a

finite positive number, which depends on K and has a limit when blocks are large $b \to \infty$. GRK is the most efficient partial search algorithm known in literature [53, 57, 59, 61, 62].

GRK can be applied in a sequence (one after another), *i.e.* after the first GRK, the target block found can be further partitioned into sub-blocks. Then a second GRK can be applied to find the sub-block containing the target item (called the *target sub-block*). We shall call the sequence of GRK's a partial search *hierarchy*. In the hierarchical search we iterate GRK. A practical example would be: In order to find a hotel, we first look at a State map and then a town map. We shall see that the second GRK works faster than the first one. Actually, GRK can be conducted repeatedly until we find the smallest target sub-sub-block interested. The total number of queries is the sum of queries of each GRK in the hierarchy. (We use number of queries as measure of complexity.)

Alternative to a partial search hierarchy which finds the target sub-sub-block, we could partition the database directly into sub-sub-blocks and use GRK once: We shall call it *direct* partial search. Although each GRK works faster than the previous one in the hierarchy, it is not guaranteed that the total number of queries in the hierarchy (sequence of GRK's) is less than that of a direct partial search. On the contrary, we will prove that direct partial search works faster, which is the main result of this chapter. For example, consider a database partitioned into 2 blocks. Each block is partitioned into 2 sub-blocks, so totally 4 sub-blocks. One could first find the target block using GRK, then the target sub-block using a sequential GRK. However, it is faster to run a GRK directly over the 4 sub-blocks, which finds the target sub-block once.

This chapter consists of six sections:

1. A introduction to the problem of database search (§ 2.1);
2. The Grover search algorithm (§ 2.2);
3. Mathematical formulation of the GRK partial search algorithm (§ 2.3);
4. A detailed study of the partial search hierarchy (§ 2.4);
5. A comparison between a hierarchical partial search with a direct partial search and proof of the main result that the direct partial search works faster (§ 2.5);
6. A brief summary (§ 2.6).

2.2 The Grover Search Algorithm

In this chapter, we will consider different methods of partial search § 2.3.1 . They are all built on the original idea of the full Grover search [41, 56, 65]. We study the Grover search in this section.

2.2.1 The Quantum Oracle

Let us formulate the problem. Consider a database of N items with one target item. [1] The database is associated with a Hilbert space with N normalized basis vectors. The basis vector corresponding to item x is denoted by $|x\rangle$. Suppose that we are equipped with a quantum oracle which has a similar ability as the classical oracle to recognize the target item. This recognition is signaled by making use of an *oracle* qubit (an auxiliary qubit also called the *working basis*). Mathematically, the oracle is a unitary operator U_f defined by its action on the computational basis:

$$U_f|x\rangle|y\rangle = |x\rangle|y \oplus f(x)\rangle, \tag{2.3}$$

where $|x\rangle$ is the address of the item in the database, $\oplus$ denotes addition modulo 2, and the oracle qubit $|y\rangle$ is a single qubit which is flipped if and only if $f(x) = 1$. The unitary operator U_f serves as the quantum version of the classical oracle, whose result depends on the value of the test function (classical oracle) $f(x) = \delta_{x,t}$. We can check whether x is a solution (target) by preparing $|x\rangle|0\rangle$, applying the oracle, and measuring the oracle qubit (working basis) to see if it has been flipped to $|1\rangle$. It is crucial that the oracle has an eigenstate $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$:

$$\begin{aligned} U_f|x\rangle\left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) &= |x\rangle\left(\frac{|0 \oplus \delta_{x,t}\rangle - |1 \oplus \delta_{x,t}\rangle}{\sqrt{2}}\right) \\ &= (-1)^{\delta_{x,t}}|x\rangle\left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \\ &= (-1)^{f(x)}|x\rangle\left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right). \end{aligned} \tag{2.4}$$

Notice that the state of the oracle qubit is not changed. If we fix the oracle qubit (working basis) at this eigenstate throughout the quantum search algorithm, this auxiliary qubit can therefore be omitted. We could effectively

[1] Target item also called in literature *marked item* or *solution*.

say

$$U_f|x\rangle = (-1)^{f(x)}|x\rangle = I_t|x\rangle, \tag{2.5}$$

so that a query to the oracle is equivalent to a reflection I_t about the plane perpendicular to the target $|t\rangle$. (Note that the form (2.5) may suggests that we actually know the target $|t\rangle$ which is not the real case.)

2.2.2 The Grover Algorithm

With the oracle well-defined, we now proceed on to the main algorithm. The Grover search is a quantum algorithm which starts from the uniform superposition of all basis vectors in the whole database:

$$|s_1\rangle = \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} |x\rangle, \qquad \langle s_1|s_1\rangle = 1. \tag{2.6}$$

The algorithm searches for a single target item $|t\rangle$ iteratively. The Grover iteration is a unitary transform:

$$G_1 = -I_{s_1} I_t. \tag{2.7}$$

Later we shall call it a *global iteration* in GRK. Here I_t and I_{s_1} are two reflections about the plane perpendicular to the target item $|t\rangle$ (this reflection corresponds to a query to the oracle) and about the plane perpendicular to the uniform superposition $|s_1\rangle$ defined in (2.6), respectively:

$$I_t = I - 2|t\rangle\langle t|, \tag{2.8}$$

$$I_{s_1} = I - 2|s_1\rangle\langle s_1|, \tag{2.9}$$

where I is the identical operator. The Grover iteration G_1, as a product of two reflections, is a rotation in the Hilbert space from $|s_1\rangle$ towards the target $|t\rangle$ by an angle $2\theta_1$ defined by [65]

$$\sin^2 \theta_1 = \frac{1}{N}. \tag{2.10}$$

This fact is straightforward to verify either through induction or by finding the eigenstates of the Grover iteration G_1. Another way to see it is this: Realizing that the amplitude of all non-target items are always the same in

the algorithm, we define

$$|nt\rangle = \frac{1}{\sqrt{N-1}} \sum_{x \neq t}^{N-1 \text{ items}} |x\rangle. \tag{2.11}$$

Then G_1 becomes a rotation in the 2-dimensional space spanned by the orthonormal basis $\{|t\rangle, |nt\rangle\}$. In this basis, $|s_1\rangle$ is represented by

$$|s_1\rangle = \begin{pmatrix} \sin\theta_1 \\ \cos\theta_1 \end{pmatrix} \tag{2.12}$$

and G_1 becomes

$$G_1 = \begin{pmatrix} \cos 2\theta_1 & \sin 2\theta_1 \\ -\sin 2\theta_1 & \cos 2\theta_1 \end{pmatrix}. \tag{2.13}$$

After j_1 iterations the state of the database becomes [41, 65]

$$G_1^{j_1}|s_1\rangle = \sin\left((2j_1+1)\theta_1\right)|t\rangle + \frac{\cos\left((2j_1+1)\theta_1\right)}{\sqrt{N-1}} \sum_{x \neq t}^{\text{N-1 items}} |x\rangle. \tag{2.14}$$

Therefore after $j_{\text{full}} = \pi/(4\theta_1) - 1/2$ iterations the probability amplitude of $|t\rangle$ becomes unity and amplitudes of other items all vanish. *i.e.*

$$G_1^{j_{\text{full}}}|s_1\rangle = |t\rangle. \tag{2.15}$$

As N becomes large $j_{\text{full}} = \pi/(4\theta_1) - 1/2$ approaches (2.1). More rigorously speaking, j_{full} may not be an integer, so that we should have

$$j_{\text{full}} = \text{CI}\left(\frac{\pi}{4\theta_1} - \frac{1}{2}\right) \tag{2.16}$$

number of iterations, where $\text{CI}(x)$ denote the integer closest to the real number x. The error is of the order $\mathcal{O}\left(\frac{1}{N}\right)$, which can be corrected by repetition. More details on Grover search can be found in Chapter 6 of [41].

2.3 The GRK Partial Search Algorithm

Now we proceed to quantum partial search in which the database is partitioned into blocks and the algorithm searches for the block containing the target item. We are particularly interested in the ideal problem that both the size of each block b and thus that of the database N become large, with their ratio (number

of blocks) $K = N/b$ fixed. *i.e.*

$$b \to \infty, \qquad N \to \infty, \qquad K = \frac{N}{b} \to \text{finite}. \tag{2.17}$$

2.3.1 Algorithms for Partial Search

Before introducing the GRK partial search algorithm (see § 2.3.2), we first look at a few other algorithms for comparison:

1. Naive Search

   Pick a block randomly and make a full Grover search in it (which makes $\frac{\pi}{4}\sqrt{\frac{N}{K}}$ queries to the oracle). If we find the target item then we understand that this is the target block. If not, then we discard this block and pick another randomly. Make a full Grover search in it and repeat this procedure till we find the target block. In the worst case the target block will be the last one. So with probability 1 we have to use

   $$r(N, K) = \frac{(K-1)}{\sqrt{K}} \frac{\pi}{4} \sqrt{N} \tag{2.18}$$

   iterations (queries) to find the target block. [2]

   A full Grover search finds the target item in $(\pi/4)\sqrt{N}$ queries. If we know the exact address of the target item then we also know the target block. Comparing $(\pi/4)\sqrt{N}$ with $r(N, K)$ in (2.18), we see that the naive version is faster only for two blocks $K = 2$. (If $K \geq 3$ a full search is faster).

2. Binary Search

   Assume that $K = 2^k$ with k being a positive integer. Divide the database into two blocks and make a full Grover search in one block. If the target item is not found, then take the remaining block and divide it into two sub-blocks. Pick a sub-block randomly and make a full search again in it. Repeat the procedure until we are left with the last block. In the worst case, the number of queries necessary to find the target block is

   $$\frac{\pi}{4}\sqrt{N}\left\{\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{4}} + \ldots + \frac{1}{2^{k/2}}\right\}, \qquad k = \log_2 K. \tag{2.19}$$

[2] $(\sqrt{K}/2)(\pi/4)\sqrt{N}$ queries on average.

The first two terms in the braces of (2.19) are greater than 1 for $K \geq 3$,

$$\frac{1}{\sqrt{2}} + \frac{1}{2} = \frac{\sqrt{2}+1}{2} > 1. \tag{2.20}$$

So this algorithm is less efficient than a full Grover search, when $K > 2$.

3. Grover and Radhakrishnan Version

   A faster version was found in [57]. Pick randomly a block and make a full Grover search in the compliment (the set of all items in the rest of the database). Either the target item (and block) is found after the search or the picked block is the target block. This requires $\frac{\pi}{4}\sqrt{b(K-1)} = \frac{\pi}{4}\sqrt{N}\sqrt{\frac{K-1}{K}}$ queries. It is faster than a full search.

2.3.2 The GRK Partial Search Algorithm

L. K. Grover and J. Radhakrishnan also discovered a faster quantum algorithm [57] for partial search which uses the same oracle as the main Grover algorithm. Partial search also starts from the uniform superposition of all basis states (2.6). A general structure of the algorithm is [53, 57, 59–62]:

Step 1. Global iterations:
j_1 standard Grover iterations (2.7). After this step the state of database is $G_1^{j_1}|s_1\rangle$.

Step 2. Simultaneous local iterations in each block:
j_2 local Grover iterations defined in (2.21) below. After step 2 the state of database is $G_2^{j_2} G_1^{j_1}|s_1\rangle$.
Local iteration is defined by

$$G_2 = \bigoplus_{\text{blocks}}^{K} G_2^{\overset{\text{one}}{\text{block}}} = -\left(\bigoplus_{\text{blocks}}^{K} I_{s_2}\right) I_t. \tag{2.21}$$

It is a direct sum of Grover iterations (called local queries) defined in each block

$$G_2^{\overset{\text{one}}{\text{block}}} = -I_{s_2} I_t. \tag{2.22}$$

In the expression I_t is the same reflection (2.8), *i.e.* query to the oracle. I_{s_2} is a local reflection

$$I_{s_2} = I - 2|s_2\rangle\langle s_2|. \tag{2.23}$$

Here $|s_2\rangle$ is the uniform superposition of items in one block

$$|s_2\rangle = \frac{1}{\sqrt{b}} \sum_{\text{one block}}^{b \text{ items}} |x\rangle. \tag{2.24}$$

Local iteration G_2 is a the Grover iteration in each block done simultaneously in all blocks. G_2 acts trivially on non-target blocks. A non-trivial operation (rotation) is present only in the target block with new rotation angle θ_2 defined by

$$\sin^2\theta_2 = \frac{K}{N} = \frac{1}{b}. \tag{2.25}$$

In other words, G_2 acts on non-target blocks as the identity; It acts on the target block as a local rotation. Note that amplitudes of all items in non-target blocks remain intact in this step.

Step 3. Location of the target block with a final global iteration [59, 61, 62]: We have to vanish amplitudes of all items in non-target blocks. It can be done by application of one more global iteration. The resulting state is

$$|d\rangle \equiv G_1 G_2^{j_2} G_1^{j_1} |s_1\rangle = \sin\omega|t\rangle + \frac{\cos\omega}{\sqrt{b-1}} \sum_{\substack{x\neq t \\ \text{target block}}}^{\substack{\text{b-1} \\ \text{items}}} |x\rangle. \tag{2.26}$$

The final state (2.26) is expressed as a superposition over items in the target block only. This is realized by requiring that the amplitude of any non-target block vanishes after the partial search, *i.e.*

$$\langle x|d\rangle = 0. \tag{2.27}$$

Here x is an arbitrary item in any non-target block. This vanishing condition can be written explicitly as an equality for j_1 and j_2, see (2.47) and [59]. We shall call it a *cancellation condition*.

The Mathematical Framework

Now let us follow the three steps above and find the cancellation condition (2.27), hence the total queries to the oracle explicitly. **Step 1** is nothing but the first j_1 iterations of the full Grover search. We make use of the same notations as in § 2.2.2 . These j_1 iterations are easily carried out by using the eigenvectors of G_1:

$$\begin{aligned} G_1|\psi_1^{\pm}\rangle &= \lambda_1^{\pm}|\psi_1^{\pm}\rangle, \qquad \lambda_1^{\pm} = \exp\left(\pm 2\mathrm{i}\theta_1\right), \\ |\psi_1^{\pm}\rangle &= \frac{1}{\sqrt{2}}|t\rangle \pm \frac{\mathrm{i}}{\sqrt{2}}\left(\sum_{\substack{x=0\\x\neq t}}^{N-1}\frac{|x\rangle}{\sqrt{(N-1)}}\right). \end{aligned} \tag{2.28}$$

After j_1 queries the state of the database is

$$G_1^{j_1}|s_1\rangle = \sin\left((2j_1+1)\theta_1\right)|t\rangle + \frac{\cos\left((2j_1+1)\theta_1\right)}{\sqrt{N-1}}\sum_{\substack{x=0\\x\neq t}}^{N-1}|x\rangle. \tag{2.29}$$

During **Step 2** local searches G_2 are made in each block separately in parallel. First let us consider the state of a non-target block at the beginning of **Step 2**:

$$|nB\rangle = a_{nt}\sum_{\text{one block}}^{b \text{ items}}|x\rangle = a_{nt}\sqrt{b}\,|s_2\rangle \tag{2.30}$$

We can read the coefficient from (2.29) that

$$a_{nt} = \frac{\cos\left((2j_1+1)\theta_1\right)}{\sqrt{N-1}} \tag{2.31}$$

The state of a non-target block does not change during the second step:

$$I_t|nB\rangle = |nB\rangle = -I_{s_2}|nB\rangle = G_2|nB\rangle. \tag{2.32}$$

Now let us consider the target block. After **Step 1** its state can be obtained from (2.29) to be

$$|B\rangle = \sin\left((2j_1+1)\theta_1\right)|t\rangle + \cos\left((2j_1+1)\theta_1\right)\frac{\sqrt{b-1}}{\sqrt{N-1}}|ntt\rangle. \tag{2.33}$$

Here the $|ntt\rangle$ is a normalized sum of all non-target items in the target block:

$$|ntt\rangle = \frac{1}{\sqrt{b-1}} \sum_{\substack{x \neq t \\ \text{target block}}}^{b-1 \text{ items}} |x\rangle, \qquad \langle ntt|ntt\rangle = 1. \tag{2.34}$$

Step 2 works as the Grover search within the target block with a different initial state. It is also convenient to construct eigenvectors of G_2 (in a similar way as the eigenvectors of G_1, see (2.28)):

$$\begin{aligned} G_2|\psi_2^\pm\rangle &= \lambda_2^\pm |\psi_2^\pm\rangle, \qquad \lambda_2^\pm = \exp\left(\pm 2\mathrm{i}\theta_2\right), \\ |\psi_2^\pm\rangle &= \frac{1}{\sqrt{2}}|t\rangle \pm \frac{\mathrm{i}}{\sqrt{2}}|ntt\rangle \end{aligned} \tag{2.35}$$

We can resolve these equations as

$$|ntt\rangle = \frac{\mathrm{i}}{\sqrt{2}}\left(-|\psi_2^+\rangle + |\psi_2^-\rangle\right), \qquad |t\rangle = \frac{1}{\sqrt{2}}\left(|\psi_2^+\rangle + |\psi_2^-\rangle\right) \tag{2.36}$$

Now we can express the state of the target block in terms of the eigenvectors of G_2:

$$\begin{aligned} |B\rangle = & \left[\frac{\sin\left((2j_1+1)\theta_1\right)}{\sqrt{2}} - \mathrm{i}\sqrt{\frac{b-1}{N-1}}\frac{\cos\left((2j_1+1)\theta_1\right)}{\sqrt{2}}\right]|\psi_2^+\rangle \\ + & \left[\frac{\sin\left((2j_1+1)\theta_1\right)}{\sqrt{2}} + \mathrm{i}\sqrt{\frac{b-1}{N-1}}\frac{\cos\left((2j_1+1)\theta_1\right)}{\sqrt{2}}\right]|\psi_2^-\rangle \end{aligned} \tag{2.37}$$

After j_2 iterations the target block will become

$$\begin{aligned} G_2^{j_2}|B\rangle = & \frac{\mathrm{e}^{2\mathrm{i}\theta_2 j_2}}{\sqrt{2}}\left[\sin\left((2j_1+1)\theta_1\right) - \mathrm{i}\sqrt{\frac{b-1}{N-1}}\cos\left((2j_1+1)\theta_1\right)\right]|\psi_2^+\rangle \\ + & \frac{\mathrm{e}^{-2\mathrm{i}\theta_2 j_2}}{\sqrt{2}}\left[\sin\left((2j_1+1)\theta_1\right) + \mathrm{i}\sqrt{\frac{b-1}{N-1}}\cos\left((2j_1+1)\theta_1\right)\right]|\psi_2^-\rangle \end{aligned} \tag{2.38}$$

As a result, we can use (2.35) to express the state of the target block in terms of the basis states

$$|B_2\rangle \equiv G_2^{j_2}|B\rangle = a_t|t\rangle + a_{ntt}|ntt\rangle \tag{2.39}$$

and to calculate the amplitudes:

$$\begin{aligned} a_t &= \cos(2j_2\theta_2)\sin\left((2j_1+1)\theta_1\right) \\ &\quad +\sqrt{\frac{b-1}{N-1}}\sin(2j_2\theta_2)\cos\left((2j_1+1)\theta_1\right), \qquad (2.40) \\ a_{ntt} &= -\sin(2j_2\theta_2)\sin\left((2j_1+1)\theta_1\right) \\ &\quad +\sqrt{\frac{b-1}{N-1}}\cos(2j_2\theta_2)\cos\left((2j_1+1)\theta_1\right). \qquad (2.41) \end{aligned}$$

Before presenting the last step, we shall emphasize that different versions of the last operation in **Step 3** of GRK appeared in literature [53, 57, 59]. People have finalized (after **Steps 1** and **2**) the state $|v\rangle \equiv G_2^{j_2}G_1^{j_1}|s_1\rangle$ with different operations I_{s_1}, $-I_tI_{s_1}$, or $G_1 \equiv -I_{s_1}I_t$. Grover and Radhakrishnan used I_{s_1} [57]. This makes one less query to the oracle but the amplitude of the target item is negative in the final state $I_{s_1}|v\rangle$. Article [59] used $-I_tI_{s_1}$ and article [62] used G_1. The last two version become the same in the large block limit. This means that final states $-I_tI_{s_1}|v\rangle$ and $G_1|v\rangle$ are equivalent (of the same form) when $b \to \infty$, though I_{s_1} and I_t do not commute in general. We choose G_1 in our formal presentation throughout this chapter because it uses the same Grover iteration. However, in the calculations below (only within the discussion of **Step 3**) we use $-I_tI_{s_1}$ instead for convenience. All statements are valid for G_1 because of the equivalence in the large block limit. Then **Step 3** consists of the following operations. We start by application of the operator

$$-I_{s_1} = -I + 2|s_1\rangle\langle s_1| \qquad (2.42)$$

(see (2.6)) to the state of the whole database. Consider an arbitrary vector

$$|v\rangle = \sum_{x=0}^{N-1} a_x|x\rangle. \qquad (2.43)$$

The operator $-I_{s_1}$ inverts the coefficients about the average:

$$-I_{s_1}|v\rangle = \sum_{x=0}^{N-1}\breve{a}_x|x\rangle, \qquad \breve{a}_x = 2\bar{a} - a_x, \qquad \bar{a} = \sum_{x=0}^{N-1}\frac{a_x}{N}. \qquad (2.44)$$

We see from (2.44) this is global inversion about average $a_x \to 2\bar{a} - a_x$. The amplitude of an item which we want to vanish should be double average: $a_x = 2\bar{a}$. We want to annihilate the amplitudes of items in non-target blocks $a_{nt} \to 0$. This means that the amplitudes introduced in the previous step

should satisfy $a_{nt} = 2\bar{a}$:

$$a_{nt} = \frac{2}{N}\left[b\ (K-1)a_{nt} + a_t + \sqrt{b-1}\ a_{ntt}\right], \tag{2.45}$$

see (2.34). We can re-write this in a form:

$$-\ N\left(\frac{1}{2} - \frac{1}{K}\right) a_{nt} = a_t + \sqrt{b-1}\ a_{ntt} \tag{2.46}$$

Substituting here the expressions (2.31), (2.40) and (2.41) we obtain the explicit *cancellation equation*:

$$\begin{aligned} & \frac{-N}{\sqrt{N-1}}\left(\frac{1}{2} - \frac{1}{K}\right)\cos\left((2j_1+1)\theta_1\right) \\ = \quad & \cos(2j_2\theta_2)\sin\left((2j_1+1)\theta_1\right) \\ + \quad & \sqrt{\frac{b-1}{N-1}}\sin(2j_2\theta_2)\cos\left((2j_1+1)\theta_1\right) \\ - \quad & \sqrt{b-1}\sin(2j_2\theta_2)\sin\left((2j_1+1)\theta_1\right) \\ + \quad & \frac{b-1}{\sqrt{N-1}}\cos(2j_2\theta_2)\cos\left((2j_1+1)\theta_1\right) \end{aligned} \tag{2.47}$$

This equation guarantees that the amplitude of each item in each non-target block vanishes:

$$\begin{aligned} I_{s_1}|nB\rangle &= 0, \\ I_{s_1}|B_2\rangle &= (a_t - a_{nt})|t\rangle + (a_{ntt} - \sqrt{b-1}\ a_{nt})|ntt\rangle. \end{aligned} \tag{2.48}$$

Here we used (2.39), (2.44) and $a_{nt} = 2\bar{a}$. Next, to prepare for a next partial search we make an extra query and turn the target block into the final state:

$$\begin{aligned} |d\rangle &= -I_t I_{s_1}|B_2\rangle = \sin\omega|t\rangle + \cos\omega|ntt\rangle \\ &= (a_t - a_{nt})|t\rangle - (a_{ntt} - \sqrt{b-1}\ a_{nt})|ntt\rangle. \end{aligned} \tag{2.49}$$

Below we shall call ω the block angle, we shall show that it depends only on number of blocks K.

Now we can perform a *measurement*. In the simplest case $N = 2^n$ and $K = 2^k$, we label blocks by k qubits (items inside of a block are labeled by $n-k$ qubits). We measure only k block qubits and find the target block.

Let us remark that we could have replaced the whole **Step 3** by application of a single global iteration G_1 to the database (see (2.7)) and make

measurement of the block qubits. The state $|d\rangle$ (2.49) of the target block before measurement is not altered in the large block limit.

The Large Block Limit

To see universal features we consider the limit when each block is very large. In the large block limit $b \to \infty$, the total number of items is also large $N \to \infty$, while the ratio $K = N/b$ is kept finite. Then the expression for rotation angles (2.10) and (2.25) simplifies:

$$\theta_1 \to \frac{1}{\sqrt{N}}, \qquad \theta_2 \to \frac{1}{\sqrt{b}}. \tag{2.50}$$

It turns out convenient to re-write numbers of iterations in a scale form [57]

$$j_1 = \left(\frac{\pi}{4} - \frac{\eta}{\sqrt{K}}\right)\sqrt{N}, \qquad j_2 = \frac{\alpha}{\sqrt{K}}\sqrt{N}. \tag{2.51}$$

Here η and α are parameters of order 1 (they have a limit). Then the arguments of trigonometric functions in (2.47) become

$$(2j_1+1)\theta_1 = \frac{\pi}{2} - \frac{2\eta}{\sqrt{K}}, \qquad 2j_2\theta_2 = 2\alpha. \tag{2.52}$$

Now the cancellation condition (2.47) takes the following form

$$\begin{aligned} & -\sqrt{Kb}\left(\frac{1}{2} - \frac{1}{K}\right)\sin\left(\frac{2\eta}{\sqrt{K}}\right) \\ = \;& \cos(2\alpha)\cos\left(\frac{2\eta}{\sqrt{K}}\right) + \frac{1}{\sqrt{K}}\sin(2\alpha)\sin\left(\frac{2\eta}{\sqrt{K}}\right) \\ & -\sqrt{b}\sin(2\alpha)\cos\left(\frac{2\eta}{\sqrt{K}}\right) + \sqrt{\frac{b}{K}}\cos(2\alpha)\sin\left(\frac{2\eta}{\sqrt{K}}\right). \end{aligned} \tag{2.53}$$

For $b \to \infty$ the leading contribution in this equation is of order $\sqrt{b}$. We can neglect contribution of the target item into the equation (first two terms in the r.h.s.). So we can simplify the equation (2.53) to

$$\begin{aligned} & \sqrt{K}\left(\frac{1}{2} - \frac{1}{K}\right)\sin\left(\frac{2\eta}{\sqrt{K}}\right) \\ = \;& \sin(2\alpha)\cos\left(\frac{2\eta}{\sqrt{K}}\right) - \frac{1}{\sqrt{K}}\cos(2\alpha)\sin\left(\frac{2\eta}{\sqrt{K}}\right). \end{aligned} \tag{2.54}$$

Therefore, the vanishing condition (2.27) and (2.47) in terms of these parameters simplifies in the large b limit as [53, 59]

$$\tan\left(\frac{2\eta}{\sqrt{K}}\right) = \frac{2\sqrt{K}\sin 2\alpha}{K - 4\sin^2\alpha}. \tag{2.55}$$

At this point, we also calculate the block angle ω in the expression for the final state of the target block (2.26) or (2.49):

$$\tan\omega = \frac{1}{2\tan\alpha} + \left(\frac{2}{K} - \frac{1}{2}\right)\tan\alpha. \tag{2.56}$$

Now we specify ranges of these parameters α and η introduced in (2.51). Because of the constraint (2.55) relating the two parameters, it is sufficient to specify the range of α. As seen from (2.26) and (2.56) that amplitudes (of items in the database after GRK) depend on $\sin(2j_2\theta_2) \sim \sin(2\alpha)$ and $\cos(2j_2\theta_2) \sim \cos(2\alpha)$. So that it is sufficient to take values of α within one period: $\alpha \in [a, a+\pi]$, with a some real number determined later. We are looking for the exact boundaries of α set by physical considerations.

Query numbers (2.51) are non-negative:

$$j_1 = \left(\frac{\pi}{4} - \frac{\eta}{\sqrt{K}}\right)\sqrt{N} \geq 0, \tag{2.57}$$

$$j_2 = \frac{\alpha}{\sqrt{K}}\sqrt{N} \geq 0. \tag{2.58}$$

Total query number $\sim (j_1 + j_2)$ (see (2.65) below) should be less than that of a full Grover search:

$$j_1 + j_2 = \left(\frac{\pi}{4} + \frac{\alpha - \eta}{\sqrt{K}}\right)\sqrt{N} \leq \frac{\pi}{4}\sqrt{N}. \tag{2.59}$$

These three inequalities (2.57), (2.58) and (2.59) yield that

$$0 \leq \alpha \leq \eta \leq \frac{\pi}{4}\sqrt{K}. \tag{2.60}$$

We use constraint (2.55) to express η as a function of α

$$\eta(\alpha) = \frac{1}{2}\sqrt{K}\,\mathrm{Arctan}\left(\frac{2\sqrt{K}\sin 2\alpha}{K - 4\sin^2\alpha}\right) \tag{2.61}$$

K	2	3	4	5	6	100	∞
$\alpha_B(K)$	$\frac{\pi}{4}$	$\frac{\pi}{3}$	$\frac{\pi}{2}$	1.22683	1.15100	0.956221	0.947747

Table 2.1: Upper Bound of α

with function Arctan(x) multi-valued. But according to (2.60), we have

$$0 \leq \text{Arctan}\left(\frac{2\sqrt{K}\sin 2\alpha}{K - 4\sin^2\alpha}\right) \leq \frac{\pi}{2}. \tag{2.62}$$

Therefore we could take the principal branch arctan (x). Now inequality (2.60) becomes

$$0 \leq \alpha \leq \frac{1}{2}\sqrt{K}\arctan\left(\frac{2\sqrt{K}\sin 2\alpha}{K - 4\sin^2\alpha}\right) \leq \frac{\pi}{4}\sqrt{K}. \tag{2.63}$$

This inequality determines range of α.

The solution of (2.60) (or (2.63) equivalently) can be written in the following form:

$$0 \leq \alpha \leq \alpha_B(K). \tag{2.64}$$

Here the upper bound $\alpha_B(K)$ is a function of K. When $K = 2$, 3 or 4, $\alpha_B(K)$ coincide with the singularities of $\eta(\alpha)$. $(K - 4\sin^2\alpha = 0$ at these singularities.) When $K \geq 5$, values of $\alpha_B(K)$ can be solved numerically. As K increases, $\alpha_B(K)$ approaches a certain positive number $\alpha_B(\infty)$. This limit $\alpha_B(\infty) = 0.947747\ldots$ is the solution of $\alpha = \sin(2\alpha)$. (Inequality $\alpha \leq \eta(\alpha)$ becomes $\alpha \leq \sin(2\alpha)$ as $K \to \infty$.) The value of $\alpha_B(K)$ always lies in between $\alpha_B(\infty)$ and $\frac{\pi}{2}$ when $K \geq 5$. We list these results in Table 2.1.

The Optimization

It is preferred that the partial search makes the least number of queries to the oracle. We discuss the optimization of the partial search algorithm in this section. (See [59] where the GRK was first optimized).

The total number of queries is

$$S(K) \equiv j_1 + j_2 + 1 \overset{b\to\infty}{\longrightarrow} \left(\frac{\pi}{4} + \frac{\alpha - \eta}{\sqrt{K}}\right)\sqrt{N}. \tag{2.65}$$

It has to be minimized subject to the constraint (2.55). The minimum number

of queries is achieved at

$$\eta\left(K\right)=\frac{1}{2}\sqrt{K}\arctan\left(\frac{\sqrt{3K-4}}{K-2}\right),\qquad\alpha\left(K\right)=\frac{1}{2}\arccos\left(\frac{K-2}{2(K-1)}\right). \tag{2.66}$$

Thus the minimized number of queries of GRK partial search (as a function of K) is

$$S\left(K\right)\overset{b\to\infty}{\longrightarrow}\left(\frac{\pi}{4}+\frac{\alpha\left(K\right)-\eta\left(K\right)}{\sqrt{K}}\right)\sqrt{N}. \tag{2.67}$$

Note that $\alpha-\eta$ is negative and number of blocks $K\geq 2$ in a non-trivial situation.

Now we prove that (2.66) is the global minimum of $\alpha-\eta$ under constraint (2.55). We have used (2.55) to express η as a function of α

$$\eta\left(\alpha\right)=\frac{\sqrt{K}}{2}\arctan\left(\frac{2\sqrt{K}\sin 2\alpha}{K-4\sin^2\alpha}\right). \tag{2.68}$$

Now we define a function

$$f\left(\alpha\right)\equiv\alpha-\eta\left(\alpha\right) \tag{2.69}$$

which we want to minimize within the range $0\leq\alpha\leq\alpha_B(K)$. We first prove that (2.66) is a local minimum of $f(\alpha)$.

1. Case $K\geq 3$

   The first derivative of $f(\alpha)$ is

   $$f'(\alpha)=\frac{16(K-1)\sin^4\alpha-4K^2\sin^2\alpha+K^2}{16(K-1)\sin^4\alpha-8K\sin^2\alpha-K^2}. \tag{2.70}$$

   It vanishes at (2.66) with $\sin^2\alpha=\frac{K}{4(K-1)}$. We calculate next the second derivative

   $$f''(\alpha)=\frac{4K\sin 2\alpha[4(K-1)(K-2)\cos^2 2\alpha+16(K-1)\cos 2\alpha+(K-2)^2(K+2)]}{[16(K-1)\sin^4\alpha-8K\sin^2\alpha-K^2]^2}. \tag{2.71}$$

   Note that the value of the denominator at (2.66) is $\frac{K^6}{(K-1)^2}$, which is strictly positive as $K\geq 3$. The numerator is also positive because both $\sin 2\alpha$ and $\cos 2\alpha$ are positive at (2.66) with $K\geq 3$. (See § 2.3.2 for the range of $\alpha(K)$.) Therefore $f'(\alpha)=0$ and $f''(\alpha)>0$ at the solution (2.66), so that (2.66) is a local minimum for $K\geq 3$.

2. Case $K = 2$

   The case that $K = 2$ is more subtle. Expression (2.66) yields that $\alpha = \frac{\pi}{4}$ and $\eta = \frac{\pi}{2\sqrt{2}}$. However, both first (2.70) and second (2.71) derivatives of $\alpha - \eta(\alpha)$ vanish at this critical point. The third derivative is non-zero: $f'''(\alpha = \frac{\pi}{4}) = -4$. So we expand function $\alpha - \eta(\alpha)$ about the critical point

$$\alpha - \eta(\alpha)|_{K=2} = -\frac{4}{3!}\left(\alpha - \frac{\pi}{4}\right)^3 + \mathcal{O}\left(\left(\alpha - \frac{\pi}{4}\right)^4\right). \tag{2.72}$$

   We see that $\alpha = \frac{\pi}{4}$ is actually a saddle point due to the non-vanishing cubic term. The form (2.72) suggests that if α goes greater than $\frac{\pi}{4}$, value of function $\alpha - \eta(\alpha)$ could be further reduced than the value at the saddle point. However, $\alpha = \frac{\pi}{4}$ is a boundary set by physical considerations (see Table 2.1). Definition of α and η in (2.51) involves query numbers j_1 and j_2, which are non-negative. Therefore $j_1 \equiv \left(\frac{\pi}{4} - \frac{\eta}{\sqrt{2}}\right)\sqrt{N} \geq 0$, *i.e.* $\eta \leq \frac{\pi}{2\sqrt{2}}$. Now if we allow α to go beyond $\frac{\pi}{4}$ and write

$$\alpha = \frac{\pi}{4} + \delta, \qquad \eta = \frac{\pi}{2\sqrt{2}} + \epsilon. \tag{2.73}$$

   Here δ and ϵ are infinitesimals, $\delta > 0$. Then constraint (2.55) requires that

$$\epsilon = \delta. \tag{2.74}$$

   So that η would be greater than the physically allowed maximal value $\frac{\pi}{2\sqrt{2}}$ and j_1 would be negative $j_1 = -\frac{\delta}{\sqrt{2}}\sqrt{N}$. This analysis showed that α can never go beyond $\frac{\pi}{4}$ and function $\alpha - \eta(\alpha)$ is minimized at this boundary. Therefore, expression (2.66) as a local minimum is also valid in the case that $K = 2$.

Now we have proved that the critical point (2.66)

$$\alpha\left(K\right) = \frac{1}{2}\arccos\left(\frac{K-2}{2(K-1)}\right) \tag{2.75}$$

is a local minimum of $f(\alpha)$. Note that $f(\alpha)$ is analytical as $0 \leq \alpha \leq \alpha_B(K)$ and there is no singularity in this range any more. Therefore we can claim that this local minimum (2.75) is also global by comparing the value of $f(\alpha)$ at (2.75) with those at the boundaries. (We always have $0 < \alpha(K) \leq \alpha_B(K)$

K	$f(0)$	$f\left(\alpha(K)\right)$	$f\left(\alpha_B(K)\right)$
2	0	$\frac{\pi}{4}\left(1-\sqrt{2}\right)\approx -0.325323$	$\frac{\pi}{4}\left(1-\sqrt{2}\right)\approx -0.325323$
3	0	-0.337098	-0.313152
4	0	-0.339837	0

Table 2.2: Comparison of values of $f(\alpha)$ at different points.

and equality holds only for $K = 2$.) We list the comparison results for $K = 2$, 3 and 4 in Table 2.2.

When $K \geq 5$, $f(0) = f(\alpha_B(K)) = 0$, while $f(\alpha(K)) < 0$. Therefore, we conclude that the critical point (2.66) or (2.75) is always the global minimum. Thus we have completed the minimization.

In the large block limit, at the minimum (2.66) the ω appeared in (2.26) takes a particular simple form [59]

$$\omega = \alpha(K), . \tag{2.76}$$

As a consequence, the state of database after GRK (2.26) or (2.49) is the following: The amplitudes of items in non-target blocks all vanish and the state of the target block is

$$|d\rangle = \sin\alpha(K)|t\rangle + \frac{\cos\alpha(K)}{\sqrt{b-1}} \sum_{\substack{x\neq t \\ \text{target block}}}^{\substack{b-1 \\ \text{items}}} |x\rangle. \tag{2.77}$$

2.3.3 Different Partitions of a Database

Before ending this section, we briefly discuss the partition of a database into blocks. A data base of N items can be partitioned into blocks in different ways. For example, items in one block may have the first 3 bits of their addresses the same for one partition or the last 3 bits the same for another partition. For a database partitioned into K blocks of equal size $b = N/K$, there are totally

$$P(N,K) = \frac{N!}{(b!)^K\, K!} \tag{2.78}$$

different ways of partition. We could use *ancilla* qubits (also called additional or auxiliary qubits) to label these partitions. As N and b both being large, we shall need

$$\log_2 P(N,K) \sim N\log_2 K - \log_2 K! \tag{2.79}$$

ancilla qubits. For example, if we have $N = 4$ items and $K = 2$ blocks, then the number of partitions is $P(4,2) = 3$ and we shall need $\log_2 3 \approx 2$ ancillas. In practice, The number (2.79) can be further reduced if we only label the partitions commonly used, not all partitions. Then we can run GRK simultaneously for those selected partitions. When a user measures ancilla qubit in his/her favorite partition, the target block will already be found by that time.

2.4 The Partial Search Hierarchy

A partial search hierarchy is a sequence of GRK's. After location of the target block, we may consider a subsequent GRK partial search: The target block is further partitioned into $\tilde{K}$ sub-blocks and we search for the sub-block containing the target item (*target sub-block*). For example we can use Google Earth to find the State of New York first on the map of USA and then make a sequential search for Stony Brook in the State map.

We shall show below that a sequential GRK can be done faster than the first GRK. The coefficient $\pi/4$ in (2.67) is replaced by a smaller number:

$$\frac{\pi}{4} \to \frac{\pi}{4} - \frac{1}{4} \arccos\left(\frac{K-2}{2(K-1)}\right). \tag{2.80}$$

Each successive GRK works faster than the previous one for two reasons. First, the new database is smaller (only one block of the previous one). Second, the initial state of the new database (2.77) can be represented in different forms (2.82) and (2.92) below. We see that for sequential GRK, the initial state is no longer a uniform superposition of basis vectors of the new database. It is an unevenly weighted superposition with emphasis on the target $|t\rangle$, see (2.82) and (2.92). In other words, the new initial state of the database is equivalent to a partially searched (though not fully searched) one. This fact was studied in [59]. It has been shown that after the first GRK the state of the target block (new database) can be written as ((2.77) re-written)

$$|d\rangle = G_1 G_2^{j_2} G_1^{j_1} |s_1\rangle = \sin\alpha(K)|t\rangle + \frac{\cos\alpha(K)}{\sqrt{b-1}} \sum_{\substack{x \neq t \\ \text{target block}}}^{\substack{b-1 \\ \text{items}}} |x\rangle. \tag{2.81}$$

We have used relation (2.76). Compared with (2.29), we see that the state

after the first GRK (2.81) takes the form

$$|d\rangle = G_1 G_2^{j_2} G_1^{j_1} |s_1\rangle = G_2^{\frac{\alpha(K)}{2}\sqrt{b}} |s_2\rangle, \tag{2.82}$$

which serves as the initial state of the sequential GRK.

For notational convenience, we use a $\sim$ to indicate variables in the sequential GRK and make the following definitions:

$$\begin{aligned}
\text{Number of items in new database}: &\quad \tilde{N} = b = \tilde{K}\tilde{b}, && (2.83)\\
\text{Uniform superposition of new database}: &\quad |\tilde{s_1}\rangle = |s_2\rangle, && (2.84)\\
\text{New global inversion}: &\quad I_{\tilde{s}_1} = I_{s_2}, && (2.85)\\
\text{New global iteration}: &\quad \tilde{G_1} = G_2, && (2.86)\\
\text{New global rotation angle}: &\quad \tilde{\theta}_1 = \theta_2, && (2.87)\\
\text{Uniform superposition of one sub}-\text{block}: &\quad |\tilde{s_2}\rangle = \frac{1}{\sqrt{\tilde{b}}} \sum_{\substack{\text{one}\\ \text{sub}-\text{block}}}^{\tilde{b}\ \text{items}} |x\rangle, && (2.88)\\
\text{New local reflection}: &\quad I_{\tilde{s_2}} = I - 2|\tilde{s}_2\rangle\langle\tilde{s}_2|, && (2.89)\\
\text{New local iteration}: &\quad \tilde{G_2} = -I_{\tilde{s}_2} I_t, && (2.90)\\
\text{New local rotation angle}: &\quad \sin^2\tilde{\theta}_2 = \frac{1}{\tilde{b}}. && (2.91)
\end{aligned}$$

Written in these notations, the initial state of new database (2.82) is equivalent to a partially searched one with $\frac{\alpha(K)}{2}\sqrt{\tilde{N}}$ new global queries, *i.e.*

$$|d\rangle = G_1 G_2^{j_2} G_1^{j_1} |s_1\rangle = \tilde{G_1}^{\frac{\alpha(K)}{2}\sqrt{\tilde{N}}} |\tilde{s_1}\rangle. \tag{2.92}$$

Steps of the sequential GRK can be written in parallel with the first GRK using new notations (2.83)-(2.91). The resultant state of target sub-block is

$$\begin{aligned}
|\tilde{d}\rangle &\equiv \tilde{G_1}\tilde{G_2}^{\tilde{j_2}}\tilde{G_1}^{\tilde{j_1}} \left(\tilde{G_1}^{\frac{\alpha(K)}{2}\sqrt{\tilde{N}}} |\tilde{s_1}\rangle\right)\\
&= \sin\tilde{\omega}|t\rangle + \frac{\cos\tilde{\omega}}{\sqrt{\tilde{b}-1}} \sum_{\substack{x\neq t\\ \text{target sub}-\text{block}}}^{\tilde{b}-1\ \text{items}} |x\rangle. \qquad (2.93)
\end{aligned}$$

Note that the vector in the parentheses is $|d\rangle$ of (2.77). We also have (similar

to (2.27))

$$\langle x|\tilde{d}\rangle = 0, \qquad \forall\, x \in \{\text{items of non} - \text{target sub} - \text{blocks}\}\,. \tag{2.94}$$

This yields cancellation condition relating $\tilde{j_1}$ and $\tilde{j_2}$ (see [59]):

$$\begin{aligned} & \frac{-\tilde{N}}{\sqrt{\tilde{N}-1}}\left(\frac{1}{2}-\frac{1}{\tilde{K}}\right)\cos\left(2\tilde{j_1}\tilde{\theta_1}+\alpha(K)\right) \\ = \;& \cos(2\tilde{j_2}\tilde{\theta_2})\sin\left(2\tilde{j_1}\tilde{\theta_1}+\alpha(K)\right) \\ & +\sqrt{\frac{\tilde{b}-1}{\tilde{N}-1}}\sin(2\tilde{j_2}\tilde{\theta_2})\cos\left(2\tilde{j_1}\tilde{\theta_1}+\alpha(K)\right) \\ & -\sqrt{\tilde{b}-1}\sin(2\tilde{j_2}\tilde{\theta_2})\sin\left(2\tilde{j_1}\tilde{\theta_1}+\alpha(K)\right) \\ & +\frac{\tilde{b}-1}{\sqrt{\tilde{N}-1}}\cos(2\tilde{j_2}\tilde{\theta_2})\cos\left(2\tilde{j_1}\tilde{\theta_1}+\alpha(K)\right). \end{aligned} \tag{2.95}$$

We introduce parameters $\tilde{\eta}$ and $\tilde{\alpha}$ defined by

$$\tilde{j_1} = \left(\frac{\pi}{4}-\frac{\alpha(K)}{2}-\frac{\tilde{\eta}}{\sqrt{\tilde{K}}}\right)\sqrt{\tilde{N}}, \qquad \tilde{j_2} = \tilde{\alpha}\sqrt{\tilde{b}}. \tag{2.96}$$

Similarly, the algorithm is also optimized [59] in the large sub-block limit: $\tilde{b}\to\infty$, $\tilde{N}\equiv\tilde{K}\tilde{b}\to\infty$. In the limit, the angles (2.87) and (2.91) simplify as

$$\tilde{\theta}_1 = \frac{1}{\sqrt{\tilde{N}}}, \qquad \tilde{\theta}_2 = \frac{1}{\sqrt{\tilde{b}}}. \tag{2.97}$$

The minimum is achieved at

$$\begin{aligned} \tilde{\eta}\left(\tilde{K}\right) &= \frac{1}{2}\sqrt{\tilde{K}}\arctan\left(\frac{\sqrt{3\tilde{K}-4}}{\tilde{K}-2}\right) = \eta\left(\tilde{K}\right), \\ \tilde{\alpha}\left(\tilde{K}\right) &= \frac{1}{2}\arccos\left(\frac{\tilde{K}-2}{2(\tilde{K}-1)}\right) = \alpha\left(\tilde{K}\right). \end{aligned} \tag{2.98}$$

Similar to (2.76), we have in the large sub-block limit

$$\tilde{\omega} = \alpha(\tilde{K}). \tag{2.99}$$

As a result the number of queries of the sequential GRK is

$$\bar{S}\left(K,\tilde{K}\right)\equiv\tilde{j}_1+\tilde{j}_2+1\overset{\tilde{b}\to\infty}{\longrightarrow}\left(\frac{\pi}{4}-\frac{\alpha(K)}{2}+\frac{\alpha\left(\tilde{K}\right)-\eta\left(\tilde{K}\right)}{\sqrt{\tilde{K}}}\right)\sqrt{\tilde{N}}. \tag{2.100}$$

In principle, sequential GRK's can be conducted successively until the smallest target sub-sub-block is found. Here arises a question on the efficiency of the hierarchical partial search, *i.e.* whether or not is a sequence of GRK's works faster than a direct GRK partial search of the smallest sub-sub-blocks. As will be shown in the following section, a direct GRK partial search makes less queries in the quantum case.

2.5 Comparison of Hierarchical Partial Search with Direct Partial Search

The partial search hierarchy forms a sequence of GRK's. It starts from searching for the largest target block and ends with searching for the smallest target sub-sub-block. On the other hand, it is also possible to partition the database directly into the smallest sub-sub-blocks and use a single GRK to find the target sub-sub-block in one time. One question of significance is whether the hierarchical search works faster than the direct search or not. This question is of practical importance and the answer turns out to be *negative*. We prove the statement by studying the first two successive GRK's in the hierarchy.

We have already derived the optimized number of queries of the first two GRK's in (2.67) and (2.100), respectively. So that the total number of queries is the sum:

$$\begin{aligned} T\left(K,\tilde{K}\right) &\equiv S\left(K\right)+\bar{S}\left(K,\tilde{K}\right) \\ &= \left\{\frac{\pi}{4}+\frac{\frac{\pi}{4}+\frac{1}{2}\alpha\left(K\right)-\eta\left(K\right)}{\sqrt{K}}+\frac{\alpha\left(\tilde{K}\right)-\eta\left(\tilde{K}\right)}{\sqrt{K\tilde{K}}}\right\}\sqrt{N}. \end{aligned} \tag{2.101}$$

On the other hand, if the database is partitioned directly into $K\tilde{K}$ blocks, a

K	$\tilde{K}$	$S(K\tilde{K})/\sqrt{N}$	$T(K,\tilde{K})/\sqrt{N}$	$(T(K,\tilde{K})-S(K\tilde{K}))/\sqrt{N}$
2	2	0.61548	0.670379	0.054899
2	3	0.646015	0.695421	0.049406
3	2	0.646015	0.721158	0.075143
2	4	0.664521	0.71289	0.048369
4	2	0.664521	0.73929	0.074769
3	3	0.671394	0.741605	0.070211

Table 2.3: Numerical Examples of Query Numbers.

direct GRK algorithm would require

$$S\left(K\tilde{K}\right) = \left[\frac{\pi}{4} + \frac{\alpha\left(K\tilde{K}\right) - \eta\left(K\tilde{K}\right)}{\sqrt{K\tilde{K}}}\right]\sqrt{N} \tag{2.102}$$

queries instead. Let us compare $T(K,\tilde{K})$ and $S(K\tilde{K})$, assuming that both $K \geq 2$ and $\tilde{K} \geq 2$.

2.5.1 Numerical Comparison of Query Numbers and Asymptotic Analysis

Before giving the complete proof, we illustrate the fact that $T > S$ (A direct partial search works faster) by looking at a few concrete examples. Here in Table 2.3 we give a few numerical examples of query numbers $S(K\tilde{K})$ and $T(K,\tilde{K})$ as well as their difference, for a better understanding. It is clear that each $T - S$ is positive in the last column.

Independently, when number of blocks and sub-blocks both being large, *i.e.* $K \to \infty$, $\tilde{K} \to \infty$, asymptotic forms of $\alpha(x)$ and $\eta(x)$ when $x \to \infty$ are obtained from (2.66) as

$$\alpha(x) \sim \frac{\pi}{6} + \frac{1}{2\sqrt{3}x} + \frac{5\sqrt{3}}{(6x)^2}, \qquad \eta(x) \sim \frac{\sqrt{3}}{2} + \frac{1}{2\sqrt{3}x} + \frac{11\sqrt{3}}{90x^2}. \tag{2.103}$$

Then the query numbers (2.101) and (2.102) take asymptotic forms using

(2.103)

$$S(K\tilde{K}) \sim \left\{\frac{\pi}{4}+\left[\frac{\pi}{6}-\frac{\sqrt{3}}{2}+\frac{1}{5\sqrt{3}(2K\tilde{K})^2}\right]\frac{1}{\sqrt{K\tilde{K}}}\right\}\sqrt{N} \quad (2.104)$$

$$T(K,\tilde{K}) \sim \left\{\frac{\pi}{4}+\left[\left(\frac{\pi}{3}-\frac{\sqrt{3}}{2}\right)-\frac{1}{4\sqrt{3}K}-\frac{19\sqrt{3}}{10(6K)^2}\right]\frac{1}{\sqrt{K}} + \left[\frac{\pi}{6}-\frac{\sqrt{3}}{2}+\frac{1}{5\sqrt{3}(2\tilde{K})^2}\right]\frac{1}{\sqrt{K\tilde{K}}}\right\}\sqrt{N}. \quad (2.105)$$

As for the difference $T-S$ of query numbers, the ratio $K/\tilde{K}$ becomes relevant in determining the asymptotic behavior. There are three possibilities:

1. If $K/\tilde{K} \to 0$, then $1/K$ is dominating, and

$$T(K,\tilde{K}) - S(K\tilde{K}) \sim \left[\left(\frac{\pi}{3}-\frac{\sqrt{3}}{2}\right)K^{-\frac{1}{2}}\right]\frac{1}{\sqrt{N}}. \quad (2.106)$$

2. If $K/\tilde{K} \to \infty$, then $1/\tilde{K}$ is dominating, and

$$T(K,\tilde{K}) - S(K\tilde{K}) \sim \left(\frac{1}{20\sqrt{3}}K^{-\frac{1}{2}}\tilde{K}^{-\frac{5}{2}}\right)\frac{1}{\sqrt{N}}. \quad (2.107)$$

3. If $K/\tilde{K} \to$ finite number, then we have the same result as (2.106).

In both the expressions (2.106) and (2.107) the coefficients of $1/\sqrt{N}$ are positive. Up to now we see that $T > S$. Now let us formally prove as a theorem (2.111) in the next section § 2.5.2 that $T > S$ in general, when $K \geq 2$ and $\tilde{K} \geq 2$.

2.5.2 General Proof of the Inequality

Now we prove that $T\left(K,\tilde{K}\right) - S\left(K\tilde{K}\right)$ is always positive in the region both $K,\ \tilde{K} \in [2,+\infty)$. In order to complete the proof we need the following two lemmas.

Lemma 2.1

$$\frac{\pi}{4}+\left(\frac{1}{2}\alpha-\eta\right)(x) > 0, \qquad \forall\ x \in [2,+\infty)\,. \quad (2.108)$$

Proof $\forall\ x \in [2, +\infty)$
The derivative $\left[\frac{\pi}{4} + \left(\frac{1}{2}\alpha - \eta\right)\right]'(x) = \frac{1}{4\sqrt{x}} f(x)$ with
$f(x) \equiv \frac{3}{\sqrt{3x-4}} - \arctan\frac{\sqrt{3x-4}}{x-2}$. While $f'(x) = \frac{-9x+8}{2x(x-1)(3x-4)^{\frac{3}{2}}} < 0$, so that $f(x)$ monotonically decreasing. Further, since that $f(2) = \frac{3}{\sqrt{2}} - \frac{\pi}{2} > 0,\ f(x) \overset{x\to+\infty}{\longrightarrow} 0$, then continuous function $f(x) > 0$ in the region. ($f(x)$ is positive at one point $x = 2$ and tends to zero as x tends to infinity. As a continuous and monotonic function, $f(x)$ can never become negative nor zero in the region.) Therefore $\left[\frac{\pi}{4} + \left(\frac{1}{2}\alpha - \eta\right)\right]'(x) > 0$, so that $\frac{\pi}{4} + \left(\frac{1}{2}\alpha - \eta\right)(x)$ is a monotonically increasing function of x. With $\frac{\pi}{4} + \left(\frac{1}{2}\alpha - \eta\right)(2) = \frac{3-2\sqrt{2}}{8}\pi > 0$, we conclude that $\frac{\pi}{4} + \left(\frac{1}{2}\alpha - \eta\right)(2) > 0$ in the region.

Lemma 2.2

$$(\alpha - \eta)(x) \text{ monotonically decreasing}, \qquad \forall\ x \in [2, +\infty). \tag{2.109}$$

Proof $\forall\ x \in [2, +\infty)$
The derivative $(\alpha - \eta)'(x) = \frac{1}{4\sqrt{x}} g(x)$ with $g(x) \equiv \frac{\sqrt{3x-4}}{x-1} - \arctan\frac{\sqrt{3x-4}}{x-2}$. While $g'(x) = \frac{1}{x(x-1)^2\sqrt{3x-4}} > 0$, so that $g(x)$ monotonically increasing. Further, since that $g(2) = \sqrt{2} - \frac{\pi}{2} < 0,\ g(x) \overset{x\to+\infty}{\longrightarrow} 0$, then continuous function $g(x) < 0$ in the region. ($g(x)$ is negative at one point $x = 2$ and tends to zero as x tends to infinity. As a continuous and monotonic function, $g(x)$ can never become positive nor zero in the region.) Therefore $(\alpha - \eta)'(x) < 0$, we conclude that $(\alpha - \eta)(x)$ is a monotonically decreasing function of x in the region.

Having proved these two lemmas, we look at the structure of $T\left(K, \tilde{K}\right) - S\left(K\tilde{K}\right)$ using (2.101) and (2.102):

$$\begin{aligned} &T\left(K, \tilde{K}\right) - S\left(K\tilde{K}\right) \\ &= \left\{ \frac{\frac{\pi}{4} + \frac{1}{2}\alpha(K) - \eta(K)}{\sqrt{K}} + \frac{\left[\alpha\left(\tilde{K}\right) - \eta\left(\tilde{K}\right)\right] - \left[\alpha\left(K\tilde{K}\right) - \eta\left(K\tilde{K}\right)\right]}{\sqrt{K\tilde{K}}} \right\} \sqrt{N}. \end{aligned} \tag{2.110}$$

Making use of **Lemma 2.1** (2.108), we see that the numerator $\frac{\pi}{4} + \frac{1}{2}\alpha(K) - \eta(K)$ of the first term appearing in the brace of (2.110) is positive for $K \geq 2$. Making use of **Lemma 2.2** (2.109) and since $K\tilde{K} > \tilde{K}$, the monotonic property of $\alpha - \eta$ ensures that $\alpha\left(\tilde{K}\right) - \eta\left(\tilde{K}\right) > \alpha\left(K\tilde{K}\right) - \eta\left(K\tilde{K}\right)$. So that the second term in the brace of (2.110) is also positive for both $K \geq 2$ and $\tilde{K} \geq 2$. Therefore the whole brace of (2.110) is positive. As a consequence, we conclude our result in the following theorem:

Theorem 2.1

$$T\left(K,\tilde{K}\right) > S\left(K\tilde{K}\right), \qquad \forall\ K,\tilde{K} \in [2,\infty)\,. \tag{2.111}$$

i.e. Hierarchical partial search makes more queries to the oracle than direct partial search. *Direct GRK partial search works faster.*

2.5.3 Hierarchy with Many GRK's

Theorem 2.1 (2.111) can be extended to the case of hierarchical search with an arbitrary number of GRK's. The direct GRK always works faster. We prove the statement as follows.

Consider a hierarchy with m GRK's. Assume that $m \geq 2$. We denote the whole operations $G_1 G_2^{j_2} G_1^{j_1}$ of each GRK by one symbol and define an operator

$$\mathcal{G} \equiv G_1 G_2^{j_2} G_1^{j_1}. \tag{2.112}$$

The hierarchical search works on the initial state $|s_1\rangle$ as

$$\mathcal{G}_m \ldots \mathcal{G}_3 \mathcal{G}_2 \mathcal{G}_1 |s_1\rangle, \tag{2.113}$$

where the sub-index denotes position of the GRK in the hierarchy (sequence). The proof can be written formally in the following way. Define the total number of queries of the hierarchy

$$T(K_1, K_2, \ldots, K_m) \equiv S(K_1) + \sum_{i=2}^{m} \bar{S}(K_{i-1}, K_i). \tag{2.114}$$

Here K_i is number of 'sub'-blocks in the i^{th} partition of database. (We denoted K_1 and K_2 by K and $\tilde{K}$ respectively in previous sections.) $S(K_1)$ is number of queries of the first GRK, and $\bar{S}(K_{i-1}, K_i)$ that of the i^{th} GRK in the hierarchy. Note that S and $\bar{S}$ are not of the same function form. S takes the form corresponding to a direct GRK (2.67):

$$S(K_1) = \left(\frac{\pi}{4} + \frac{\alpha(K_1) - \eta(K_1)}{\sqrt{K_1}}\right)\sqrt{N}. \tag{2.115}$$

While (for $i \geq 2$) $\bar{S}$ takes a form of sequential GRK similar to (2.100):

$$\bar{S}(K_{i-1}, K_i) = \left(\frac{\pi}{4} - \frac{\alpha(K_{i-1})}{2} + \frac{\alpha(K_i) - \eta(K_i)}{\sqrt{K_i}}\right)\frac{\sqrt{N}}{\sqrt{\prod_{j=1}^{i-1} K_j}}. \tag{2.116}$$

(We denoted $S(K_1)$ and $\bar{S}(K_1, K_2)$ by $S(K)$ and $\bar{S}(K, \tilde{K})$ respectively in previous sections.) Let us substitute these expressions into (2.114):

$$T(K_1, K_2, \ldots, K_m)$$
$$= \left\{ \frac{\pi}{4} + \sum_{i=1}^{m-1} \frac{\frac{\pi}{4} + \frac{1}{2}\alpha(K_i) - \eta(K_i)}{\sqrt{\prod_{j=1}^{i} K_j}} + \frac{\alpha(K_m) - \eta(K_m)}{\sqrt{\prod_{i=1}^{m} K_i}} \right\} \sqrt{N}. \tag{2.117}$$

On the other hand, if we partition the database directly into the smallest sub-blocks, then the number of these sub-blocks would be $\prod_{i=1}^{m} K_i$. A direct GRK will locate the smallest target sub-block. This would require

$$S\left(\prod_{i=1}^{m} K_i\right) = \left\{ \frac{\pi}{4} + \frac{\alpha(\prod_{i=1}^{m} K_i) - \eta(\prod_{i=1}^{m} K_i)}{\sqrt{\prod_{i=1}^{m} K_i}} \right\} \sqrt{N} \tag{2.118}$$

queries to the oracle. Therefore the difference of (2.117) and (2.118) is

$$T\left(K_1, K_2, \ldots, K_m\right) - S\left(\prod_{i=1}^{m} K_i\right) \tag{2.119}$$
$$= \left\{ \left(\sum_{i=1}^{m-1} \frac{\frac{\pi}{4} + (\frac{1}{2}\alpha - \eta)(K_i)}{\sqrt{\prod_{j=1}^{i} K_j}} \right) + \frac{(\alpha - \eta)(K_m) - (\alpha - \eta)(\prod_{i=1}^{m} K_i)}{\sqrt{\prod_{i=1}^{m} K_i}} \right\} \sqrt{N}.$$

We will show that this expression is always positive when each $K_i \geq 2$. Using **Lemma 2.1** (2.108), we see that each term under the summation of (2.119) is positive. Using **Lemma 2.2** (2.109), $\alpha - \eta$ is a monotonically decreasing function. Note that product of all K_i's is larger than K_m, we see that the remaining term in the brace of (2.119) is also positive. Consequently, we conclude our result in the following corollary:

Corollary 2.1

$$T\left(K_1, K_2, \ldots, K_m\right) > S\left(\prod_{i=1}^{m} K_i\right), \qquad \forall\ K_i \in [2, +\infty). \tag{2.120}$$

i.e. A hierarchy of an *arbitrary* number of GRK's makes more queries to the oracle than a direct GRK. *Direct GRK partial search always works faster.*

2.6 Summary

This chapter studies quantum search. Built from the Grover search algorithm, the optimized partial search algorithm called GRK is discussed. We

have studied a partial search hierarchy and compared it with a direct partial search (GRK). Consider a database of N items with a single target item. The database is partitioned into K blocks, each block further partitioned into $\tilde{K}$ sub-blocks. Hierarchical search is that we use GRK and sequential GRK to find the target block and target sub-block, respectively. Successive GRK's can be made if the database is further partitioned. Each sequential GRK in the hierarchy works faster than the previous one. However, the total number of queries to the oracle adds up. The main conclusion is that *a partial search hierarchy works slower than a direct partial search*, see **Theorem 2.1** (2.111) and **Corollary 2.1** (2.120). For example, consider a database partitioned into 3 blocks. Each block is further partitioned into 3 sub-blocks, so totally there are 9 sub-blocks. One could first find the target block using GRK, then the target sub-block by a sequential GRK. Nevertheless, it is faster to run a GRK partial search directly over the 9 sub-blocks and find the target sub-block once.

Note: Only the class of algorithms using the standard Grover oracle was considered in the chapter. This means that if one has already built the main Grover algorithm experimentally, then we do not need any new hardware to run the GRK algorithm. Another advantage of using the same oracle I_t as the main Grover algorithm is more subtle: We can use *ancilla* (additional or auxiliary) qubits to label different partitions of the database into blocks of equal size $b = N/K$. Then we are able to run GRK algorithm simultaneously for different partitions. (See § 2.3.3 for more details.) Later a user can measure the ancilla qubits and choose his or her favorite partition, by that time the target block already will be found.

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