

DOKUZ EYLÜL UNIVERSITY
GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

**THE GENERAL APPLICATION OF THE
QUANTUM MONTE CARLO METHOD TO SPIN
SYSTEMS**

by
Ulvi KANBUR

July, 2021
İZMİR

THE GENERAL APPLICATION OF THE QUANTUM MONTE CARLO METHOD TO SPIN SYSTEMS

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**by
Ulvi KANBUR**

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Ph.D. THESIS EXAMINATION RESULT FORM

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Ulvi KANBUR

THE GENERAL APPLICATION OF THE QUANTUM MONTE CARLO METHOD TO SPIN SYSTEMS

ABSTRACT

In this thesis, we mainly study a general Monte Carlo technique for simulating spin models with quantum mechanical interactions either at finite or zero temperatures. From the two dominating simulation techniques the so-called stochastic series expansion method is challenging the other major method path integral quantum Monte Carlo in recent years. The theoretical and technical details of the stochastic series expansion quantum Monte Carlo technique consist of the main body of this thesis. The simulation technique is formulated in a general manner and the technical details are illustrated in the scope of the isotropic spin-half models without external fields for both the ferromagnetic and antiferromagnetic interactions. Complete pseudocodes are given with detailed explanations and benchmark results are compared with exact diagonalization calculations. We briefly mention the ideas of spin systems, critical phenomena, and basics of Monte Carlo that are minimally required for a solid understanding of the simulation technique at the algorithmic level. The simulation technique is applied to two physical systems. The thermal properties of a two-leg spin ladder model with a bond disorder are investigated and interestingly a crossing point is monitored for uniform susceptibility and specific heat, separately. Finally, a three-dimensional system with a disorder is reviewed as evidence of the strength of the simulation technique in exploring the critical and universal properties. The technical details will serve as a concrete background to easily extend the underlying algorithm to include a variety of models.

Keywords: Quantum Monte Carlo, stochastic series expansion, spin systems, Heisenberg model, phase transitions, universality, ladder systems, disorder systems

KUANTUM MONTE CARLO YÖNTEMİNİN SPİN SİSTEMLERİNE GENEL UYGULAMASI

ÖZ

Bu tezde temel olarak sonlu ya da sıfır sıcaklıklarda quantum mekaniksel etkileşimleri olan spin sistemlerini simüle etmek için genel bir kuantum Monte Carlo yöntemini çalıştık. İki baskın simülasyon tekniğinden biri olan ve rastgele seri açılımı olarak adlandırılan yöntem diğer yöntem olan çizgi integrali Monte Carlo yöntemine son yıllarda üstünlük sağlamıştır. Rastgele seri açılımı kuantum Monte Carlo tekniğinin teorik ve teknik detayları bu tezin ana gövdesini oluşturmaktadır. Simülasyon tekniğinin formülasyonu genel bir şekilde verilmiştir ve teknik ayrıntılar hem ferromanyetik hem de antiferromanyetik etkileşimler için dış alan içermeyen yarım spinli izotropik modeller kapsamında gösterilmiştir. Bütün sözde kodlar ayrıntılı açıklamalarla birlikte verilmiştir ve kıyaslama sonuçları tam köşegenleştirme hesaplamaları ile karşılaştırılmıştır. Simülasyon tekniğinin algoritmik seviyede iyi bir şekilde anlaşılması için minimum düzeyde gerekli olan spin sistemleri, kritik davranış ve Monte Carlo'nun temelleri hakkında kısaca bahsedilmiştir. Simülasyon tekniği iki fiziksel sisteme uygulanmıştır. Bağ bozukluğu olan iki ayaklı bir spin merdiven modelinin ısısal özellikleri araştırılmış ve ilginç bir şekilde düzgün duyarlılık ve ısı sığası için ayrı ayrı bir kesişim noktası gözlenmiştir. Son olarak, kritik ve evrensel özellikleri anlamada simülasyon tekniğinin gücünün kanıtı olarak, bozukluk içeren üç boyutlu bir sistem incelenmiştir. Teknik ayrıntılar, temel algoritmayı çeşitli modelleri içerecek şekilde kolayca genişletmek için somut bir arka plan görevi görecektir.

Anahtar kelimeler: Kuantum Monte Carlo, rastgele seri açılımı, spin sistemleri, Heisenberg modeli, faz geçişleri, evrensellik, merdiven sistemler, bozuk sistemler

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CHAPTER ONE

INTRODUCTION

Low-dimensional spin systems whether they are classical or quantum play an important role in understanding the physics behind the phenomena such as magnetism and superconductivity in the field of condensed matter. Historically, the one-dimensional (1D) Ising model has been proposed as a magnetic model (Mikeska & Kolezhuk, 2004), for which the partition function can easily be written down exactly. The quantum counterpart of the 1D Ising model, the so-called quantum Heisenberg chain, has also been solved exactly (Parkinson & Farnell, 2010) but not as easy as its classical version. Although one of the advantages of spin systems is the simplicity of being proposed as a prototypical model that might well resemble a real material, the complexity of dealing with it increases drastically depending on the parameters such as dimension and interaction types. The most prominent example is Onsager's exact solution of two-dimensional (2D) Ising model which is thought of as a monument of theoretical physics and it has the peculiarities like to be the first solved model revealing a phase transition and showing signs of universality (Baxter, 1982; Bhattacharjee & Khare, 1995).

Another important progress concerning spin systems has been the celebrated Hohenberg-Mermin-Wagner theorem which states that spontaneously broken continuous symmetries are ruled out at finite temperatures in one and two dimensions with short-range interactions (Chakravarty et al., 1989; Nachtergaele, 2006). However, a divergent susceptibility in the absence of a spontaneous magnetization has been detected in the 2D classical planar Heisenberg model and the explanation of this intriguing phenomenon has born the terms topological order or topological phase transitions (Jr et al., 1985; Readt et al., 1984). This transition has a direct connection to the other major subjects of condensed matter physics such as superfluidity or superconductivity. The two mentors of this invention John Kosterlitz and David Thouless has shared the 2016 Physics Nobel Prize with Duncan Haldane who conjectured the presence or absence of an energy gap in quantum spin chains for integer or half-integer spins, respectively (Bietenholz & Gerber, 2016).

The first exception to universality has come out in the eight-vertex model solved by Baxter which has been another breakthrough step in the theory of phase transitions and critical phenomena (Baxter, 1982; Šamaj & Bajnok, 2013). Vertex-models are significant due to their link to quantum Heisenberg models (Barma & Shastri, 1978; Baxter, 1971; Lagendijk & De Raedt, 1982) and that property encouraged researchers to develop new computational techniques such as loop algorithms to simulate (quantum) spin systems (Evertz et al., 1993).

Early theoretical studies on spin systems in one and two dimensions have aimed to find critical properties of three-dimensional (3D) models that have been thought to be more realistic. On the experimental side, the observation of a compound called $(\text{CH}_3)_4\text{NMnCl}_3$ (TMMC) by neutron scattering measurements resulted in good agreement to a classical Heisenberg antiferromagnetic model with effective spin $S = 5/2$ in one dimension (Jongh, 1990). This surprise development has further increased the interest in low-dimensional systems. Even, the Haldane's conjecture has been confirmed in the $S = 1$ chain $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2\text{ClO}_4$ (NENP) (Ma et al., 1992; Renard et al., 1987). The vital interest in low-dimensional spin systems has begun after the realization that one of the best 2D antiferromagnets, pure La_2CuO_4 is a high- T_c superconductor when doped (Jongh, 1990). This link between the spin systems and superconductivity has attracted researchers to the subject and current research problems of quantum spin systems span a large area ranging from optical lattices to quantum information theory.

As mentioned above, while the quantum spin systems are simple and powerful models to explain real materials they are complex enough to be resolved theoretically up to some precision. Various theoretical methods since the Bethe ansatz have been used to predict quantum spin systems' thermal and ground-state properties. Each method has its drawbacks and gives approximate results except for few models. Numerical calculations and simulations are inevitable in this sense and the most widely used methods in spin systems are the exact diagonalization (ED), density matrix renormalization group (DMRG), and quantum Monte Carlo (QMC) calculations. Although quantum mechanics is an eigenvalue problem, why a single numerical method based on the linear algebra is not sufficient to analyze the physical properties of systems? While the numerical methods

evolved in their strength parallelly with analytical ones, the power of computers did not. The ED method can reach all the sectors of the partition function at all temperatures but the exponential increase of the dimension of Hilbert space even with two degrees of freedom limits the computations to a very small system sizes due to insufficient computer memory. So we should be smart rather than strong and researchers have developed more clever algorithms day by day. The best approach to deal with this giant dimensionality is the Monte Carlo (MC) methods that are also too diverse with a long history and have applicability from physics to finance.

While we can trace the origin of MC methods well before the invention of computers, the breakthrough step has been the Metropolis algorithm in the field of statistical mechanics (Gubernatis, 2003; Metropolis et al., 1953). Numerical simulations such as variational and diffusion QMC methods have been used to calculate the zero-temperature properties in quantum systems since the early days of computers. A finite temperature QMC technique based on the Trotter formula (Suzuki, 1976) has been firstly tested on quantum spin systems (Suzuki et al., 1977). However, Handscomb (1962) had already proposed and applied the first finite temperature QMC method that based on the series expansion of the partition function (Handscomb, 1964). Due to the applicability of the Handscomb's method in its initial form to limited models, the Trotter-Suzuki approach has been used widely and successfully to simulate lattice models. Most QMC algorithms have variants for continuum models, especially for the ground-state calculations. Sandvik and Kurkijärvi (1991) have revitalized the Handscomb's method based on the previous improvements and later the method has been named as stochastic series expansion (SSE) QMC.

Like all methods, QMC techniques have also a flaw, they suffer from the sign problem. However, this is not a limitation to the accuracy of the results for sign-free models but to the model itself directly. Although the error stemming from the sign problem can be controlled (Sandvik, 1994) or even eliminated (Honecker et al., 2017) depending on the system and parameters, it is one of the obstacles in computational physics. As the title of the thesis suggests we will focus on quantum spin systems that are lattice models and even in this restricted subject there can be used a great number of

QMC methods. With the advent of the loop (Evertz, 2003), operator loop (Sandvik, 1999), worm (Prokof'ev et al., 1998), and directed loop (Syljuåsen & Sandvik, 2002) algorithms, the two QMC methods, namely, the path integral QMC (PIMC) and SSE QMC have evolved into their modern versions. These methods have become prominent in simulating quantum spin systems at finite and zero temperatures and both have a similar formulation. For historical reasons mentioned above the PIMC technique has been used widely in simulating quantum spin systems but the SSE QMC method has been very demanding recently due to the efficiency and straightforward implementation advantages. So this thesis will mainly focus on the SSE QMC method that is an exact and general method to simulate sign-free quantum spin systems in any dimension and geometry at finite and zero temperatures. Although the modern versions of variational and projector QMC methods (Sandvik & Evertz, 2010) are well suited for ground-state calculations the SSE QMC method will work nearly for all purposes in a robust way.

This thesis is divided into five parts. The first part including this introduction covers some abstract and necessary background to understand the QMC methods and their applications that are given in the following parts. The following chapter will include the basics of the SSE QMC method together with the formulation, application, and implementation details. In the third chapter, the SSE QMC method will be applied to a two-leg ladder spin system with a disorder and interesting results reported. The fourth chapter includes the universality results of a 3D system with a disorder. A summary of important concepts is concluded in the fifth chapter.

1.1 Quantum Spin Systems

The way to macroscopic magnetism is hidden in the purely quantum mechanical intrinsic property of matter the so-called spin. But magnetic interactions due to spin are not so strong for a spontaneous ordering at room temperatures and the real sources of collective magnetism are the purely quantum mechanical and *electrostatic* exchange interactions that are connected to spin via the Pauli exclusion principle. In magnetic systems with localized moments, the interplay of the exchange interactions is very well described by the Heisenberg model. The model is best suited for magnetic insulators

which are described by an interaction of type *superexchange* and it is defined with the following *effective* Hamiltonian,

$$H = \sum_{i,j} J_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j \quad (1.1)$$

where $J_{i,j}$ contains complicated symmetric ($J_{i,j} = J_{j,i}$, $J_{i,i} = 0$) exchange interactions as parameters and $\mathbf{S}_i$ are spin angular momentum operators at sites i on a lattice. In a system of N spins, a state is written most conveniently in the z -basis that a spin operator can act on:

$$|\alpha\rangle = |S_1^z, S_2^z, \dots, S_i^z, \dots, S_N^z\rangle.$$

where $S_i^z = -S_i, -S_i + 1, \dots, S_i$ are the spin quantum numbers in the z -basis. For $S_i = 1/2$ the following conventions can be used interchangeably: $S_i^z = -1/2, +1/2$ or $S_i^z = \downarrow, \uparrow$ or $S_i^z = -, +$ or $S_i^z = \circ, \bullet$. For an abstract notation, the same symbols will be used for both operators and corresponding eigenvalues, which will be differentiated easily by looking at their positions in the equations. The standart spin algebra gives the following eigenvalue equations:

$$S_i^z |S_1^z, S_2^z, \dots, S_i^z, \dots, S_N^z\rangle = S_i^z \hbar |S_1^z, S_2^z, \dots, S_i^z, \dots, S_N^z\rangle \quad (1.2a)$$

$$S_i^2 |S_1^z, S_2^z, \dots, S_i^z, \dots, S_N^z\rangle = S_i(S_i + 1)\hbar^2 |S_1^z, S_2^z, \dots, S_i^z, \dots, S_N^z\rangle \quad (1.2b)$$

where S_i^z is both the spin operator in the z -direction and the spin angular momentum quantum number, on the left- and right-hand side of the Eq. (1.2a), respectively. The operators between different sites always commute so the commutation relations will be given only for operators on the same site. As $|\alpha\rangle$ is an eigenket of both operators S_i^z and S_i^2 they commute, i.e., $[S_i^z, S_i^2] = 0$. Two other important operators are,

$$S_i^\pm = S_i^x \pm iS_i^y \quad (1.3)$$

where $S_i^+(S_i^-)$ is the raising (lowering) operator defined in terms of the x - and y -components of $\mathbf{S}_i$. While the orbital angular momentum quantum number can change for any given particle the spin angular momentum quantum number of a particle at site i is fixed. With keeping this in mind, the raising and lowering operators can be

applied to the basis ket $|\alpha\rangle$ in a notational consistency as follows:

$$S_i^\pm |S_1^z, \dots, S_i^z, \dots, S_N^z\rangle = \hbar \sqrt{S_i(S_i + 1) - S_i^z(S_i^z \pm 1)} |S_1^z, \dots, S_i^z \pm 1, \dots, S_N^z\rangle. \quad (1.4)$$

The following commutation relations can be deduced:

$$[S_i^\alpha, S_i^2] = 0 \quad (1.5)$$

$$[S_i^\alpha, S_i^\beta] = i\hbar \epsilon_{\alpha\beta\gamma} S_i^\gamma \quad (1.6)$$

$$[S_i^+, S_i^-] = 2\hbar S_i^z \quad (1.7)$$

$$[S_i^\pm, S_i^z] = \mp \hbar S_i^\pm \quad (1.8)$$

where α, β, γ are the Cartesian components x, y, z . The Heisenberg model is mostly studied with short-range interactions such as the nearest-neighbors (NN) or the next nearest-neighbors (NNN) and can be written in the following conventional form that includes field and anisotropy terms, also known as XXZ model,

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{i,j} \left[\Delta S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \right] - \sum_i h_i S_i^z \quad (1.9)$$

where $\langle \dots \rangle$ denotes a sum over NN, and Δ and h_i are anisotropy and field terms, respectively. However, the Hamiltonian could be written in more general the fully anisotropic form, the so-called XYZ model, which the QMC simulation technique will also include but the applications will be restricted to the Eq. (1.9) and its special limits, for compactness. Importantly, total spin operator $\mathbf{S} = \sum_i \mathbf{S}_i$ commutes with the isotropic ($\Delta = 1$) Hamiltonian in the absence of a field ($h_i = 0$), and the z -component S^z of the total spin operator commutes with the full Hamiltonian $\mathcal{H}$, thus while all the components of the magnetization are preserved for the former case only the z -component is conserved for the latter case. Namely,

$$[\mathcal{H}(\Delta = 1, h_i = 0), \mathbf{S}] = 0 \quad (1.10a)$$

$$[\mathcal{H}, S^z] = 0. \quad (1.10b)$$

The exchange, anisotropy, and field parameters determine the fate of a system together with the dimensionality of spin and space. Depending on these parameters a spin system

may exhibit different phases characterized by a cleverly defined order parameter that is finite in the ordered phase and vanishes otherwise. If $\mathbf{S}_i$ were treated as classical variables the ordered phase could be described by a helical ground-state spin configuration that minimizes $\mathcal{H}$, on a Bravais lattice. The form of the order parameter depends on the intervals of interaction variables, e.g., the sign of $J_{i,j}$. Except for the ferromagnetic ground state, the order parameter does not commute with the Hamiltonian $\mathcal{H}$ and the classical values of the order parameter are suppressed by the quantum fluctuations. As an example, on a bipartite lattice, while the antiferromagnetically ordered (Néel) state $|\uparrow\downarrow\uparrow\cdots\rangle$ is not an eigenstate of $\mathcal{H}$, the ferromagnetically ordered state $|\uparrow\uparrow\uparrow\cdots\rangle$ is an eigenstate. The order parameter for antiferromagnetic interactions called staggered magnetization is given as

$$\mathbf{m}_s = \frac{1}{N} \sum_i^N \varphi_i \mathbf{S}_i \quad (1.11)$$

where the phase factor $\varphi_i = \pm 1$ has opposite signs on each sublattice of the bipartite lattice. In simulations, the ordered states can be realized in arbitrary directions summing the vectors $\mathbf{m}_s$ to zero on average, instead, the scalar variables $\langle m_s^2 \rangle$ or $\langle |m_s| \rangle$ is computed. In a QMC simulation, different quantities can be measured such as susceptibility or specific heat for which the estimators will be given in connection with the SSE formalism. The values of the system parameters can drive a system into different phases, e.g., from a Néel state to a valence bond state (VBS). These phases are separated by well-defined sets of critical system values that compose the phase diagram of the relevant model. The description of transitions between these phases is not so simple but the behavior is universal depending just on the dimensionality and symmetry of the physical system.

The first part of the Hamiltonian $\mathcal{H}$ consists of two spin interaction operators and the second part is a field term,

$$H_{i,j} = J_{i,j} \left(\Delta S_i^z S_j^z + \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \right) - h_i S_i^z. \quad (1.12)$$

In the z -basis, only the z -components of the operator $H_{i,j}$ contribute to the diagonal matrix elements of $\mathcal{H}$ and the fluctuating part constructs the off-diagonal elements that can also be zero. For the special $S_i = 1/2$, isotropic ($\Delta = 1$, $J_{i,j} = J$), and $h_i = 0$ case, two interacting spins have eigenvalues $J/4$, $J/4$, $J/4$, $-3J/4$ that correspond to

triplet and singlet states for the first three and the last one, respectively. Here for $J < 0$ ($J > 0$) the lowest energy is $J/4$ ($-3J/4$) and the ground state is (anti)ferromagnetic with two spins (anti)parallel. In magnetic crystals, a large number of spin magnetic moments can align collectively for example in a (anti)ferromagnetic fashion and this order can be reduced by thermal fluctuations. In the thermodynamic limit, above a critical temperature, the order is completely absent and a paramagnetic state forms. This critical temperature, T_c (T_N), is known as Curie (Néel) temperature for an (anti)ferromagnet.

1.2 Phase Transitions and Scaling in Quantum Spin Systems

Phase transitions are experienced in our everyday life such as between ice and water. Another example is the ferromagnetic materials that have hundreds of Kelvin Curie temperature beyond which they are paramagnetic. The former example is a first-order transition under normal conditions and the latter is a second-order or continuous phase transition. Both of these are classical phase transitions driven by thermal fluctuations. A quantum phase transition (QPT) that is controlled by a parameter included in the Hamiltonian, $\mathcal{H}(g)$, occurs only at absolute zero temperature and is driven by quantum fluctuations via the Heisenberg uncertainty principle. Quantum phase transitions are associated with the nonanalyticities in the ground state energy of an infinite size system arising from a level-crossing mechanism (Sachdev, 2011). The classical phase transitions are well described by the Landau-Ginzburg-Wilson (LGW) paradigm that also governs the QPTs up to some context. As an example, Néel - VBS transition of the 2D $S = 1/2$ square lattice antiferromagnet is beyond the LGW paradigm (Senthil, Balents, Sachdev, Vishwanath, & Fisher, 2004; Senthil, Vishwanath, et al., 2004; Senthil et al., 2005).

After the advent of the renormalization group (RG) theory the concepts scaling, critical exponent, and universality that characterize a phase transition have fit together. Continuous phase transitions are of importance and the following ideas are given for them in an informal way to be concise. Phase transitions in principle are treated as power-law phenomena near the critical point and those notions compose the critical phenomena. A fundamental key concept of a phase transition is the correlation length that diverges near a critical point in an infinite size system. The power-law form of the

correlation length near a critical point is given as follows,

$$\xi \propto |t|^{-\nu} \quad (1.13)$$

where t is a reduced dimensionless parameter, and ν is the correlation length critical exponent. Critical exponents share the same values for different physical systems depending only on the dimensionality and the symmetry of the system, as stated in the preceding section, and this fact is known as *universality*. Scaling laws can be captured from the RG theory in the form they were historically hypothesized. If we borrow the transformation of the singular part of the free energy density, in the language of RG with two relevant parameters, we can easily extract the scaling relations (Goldenfeld, 2018). Namely,

$$f(t, h) = l^{-d} f(tl^{y_t}, hl^{y_h}) \quad (1.14)$$

where t and h are two parameters that are re-scaled under an RG transformation with exponents y_t and y_h (or the relevant eigenvalues l^{y_t} and l^{y_h} of the transformation matrix), respectively, by a factor of number of block sites l (not necessarily integer) in each spatial dimension d . Choosing $tl^{y_t} = 1$ we obtain the scaling function,

$$f(t, h) = t^{d\nu} f(1, ht^{-\Delta}) \quad (1.15)$$

with traditional exponents $1/y_t = \nu$ and $y_h/y_t = \Delta$. Due to the homogeneity of the singular part of free energy, the derivatives of f with respect to the parameters t , and h will be proportional to f itself. Thus, the second derivative of f with respect to t is proportional to $t^{d\nu-2} = t^{-\alpha}$ giving the specific heat exponent α , and similarly, the first (second) derivative of f with respect to h is proportional to $t^{d\nu-\Delta} = t^\beta$ ($t^{d\nu-2\Delta} = t^{-\gamma}$) giving the magnetization (susceptibility) exponent β (γ),

$$2 - \alpha = d\nu \quad (1.16a)$$

$$2 - \alpha - \Delta = \beta \quad (1.16b)$$

$$2 - \alpha - 2\Delta = -\gamma. \quad (1.16c)$$

Other exponent identities can be derived and the values of exponents can be obtained

from the two independent ones.

The RG procedures are not directly applicable to the systems that are described by quantum statistical mechanics due to the inseparability of the quantum partition function (Cardy, 1996). The scaling relations are valid for QPTs through the mapping of a d -dimensional quantum system into an effective classical system in $d + 1$ dimensions, in that case, the hyperscaling relations, i.e., those contain d , are replaced by $d \rightarrow d + 1$. One caveat about the hyperscaling relations is that they are not valid above an upper critical dimension that depends on the system of interest (Li et al., 1995). This quantum-classical mapping also serves as the fundamental starting point of QMC methods that will be covered in the following chapters. The extra dimension imaginary time goes into scaling functions as a finite relevant variable that mimics the crossover theory of finite size scaling (FSS) that will be discussed in the following. The phase diagrams of quantum systems can thus be constructed, and the infinite size imaginary time extra dimension, together with the other spatial d dimensions, corresponds to a zero-temperature quantum system. A schematic phase diagram can be sketched as in Figure 1.1 in which there is only one quantum critical point (QCP) and an infinite number of classical critical points that lie on the solid line and all the behavior near this line in the shaded region is of purely classical. For systems that the Hohenberg-Mermin-Wagner theorem forbids an ordered phase at finite temperatures, this line lies on $T = 0$ without any shaded region and ends at a QCP. The quantum critical region in which the quantum and thermal fluctuations are important even at comparatively high temperatures is interesting both from the theoretical and experimental points of view (M. Vojta, 2003).

1.2.1 Finite Size Scaling

Phase transitions do not take place at finite dimensions, which also seems as a restriction for the numerical methods. FSS hypothesis turns out this limitation to an advantage. At any finite dimension, the peak of a critical singular behavior will be broadened and shift, and this information is used to extract the infinite size system properties. RG theory treats the finite-size effects as a crossover phenomenon by

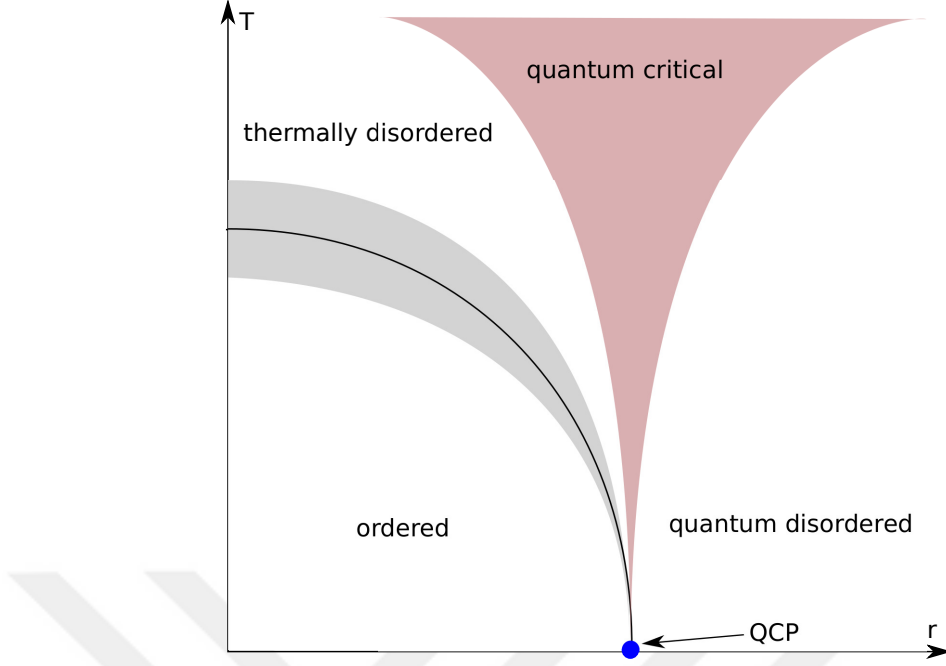


Figure 1.1 Schematic phase diagram near a QCP

incorporating the inverse system size as a relevant variable. As before,

$$f(t, h, L^{-1}) = l^{-d} f(tl^{y_t}, hl^{y_h}, L^{-1}l^{y_L}) \quad (1.17)$$

where $y_L = 1$ due to the fact that all the lengths are already reduced by a factor of l in an RG transformation. The same procedure of producing the scaling relations applies but this time it is set $L^{-1}l = 1$ to cancel out the L dependence. After replacing and putting the conventional exponents,

$$f(t, h, L^{-1}) = L^{-d} f(tL^{1/\nu}, hL^{\Delta/\nu}, 1). \quad (1.18)$$

Scaling forms of the related quantities are found by the respective derivatives of the function f as before and using the relations in Eq. (1.16). The scaling forms for the zero-field susceptibility and the specific heat are found,

$$Q \propto L^{\kappa/\nu} \partial_{xx} f(tL^{1/\nu}, hL^{\Delta/\nu}, 1) \quad (1.19)$$

where Q stands for the quantity of interest and $\kappa = \gamma, \alpha$, and $x = h, t$, respectively. For the correct values of the exponents κ and ν the data obtained for different system sizes

(not too small) collapse if one sketches $QL^{-\kappa/\nu}$ versus $tL^{1/\nu}$. More generally, the n th derivative of the free energy density ($f^{(n)}$) with respect to one of its variables gives the n th cumulant *per site* of the corresponding conserved quantity. Thus importantly, the normalized cumulants such as Binder ratios are of size independent.

1.2.2 Scaling Corrections

In practice, it is difficult to reach the asymptotic behavior and extract the critical values due to the limited linear sizes of the simulated systems that are on the order of ten or a hundred. For that reason the FSS analysis requires corrections and the answer is again hidden in the RG formalism. The idea is that the scaling functions can include an infinite number of *irrelevant* scaling fields that are negligible at the critical regime $t \rightarrow 0$. Now we write the Eq. (1.19) in a general manner for any singular quantity Q and the corresponding scaling function $\mathcal{F}$ with one relevant and one irrelevant scaling field,

$$Q(\delta, L) = L^{\kappa/\nu} \mathcal{F}(\delta L^{1/\nu}, \lambda L^{-\omega}) \quad (1.20)$$

where $\delta = g - g_c$ is a control parameter measures the distance away from the critical point g_c , λ is the leading irrelevant scaling field and $\omega > 0$ is the corresponding exponent. If we use a size-independent singular quantity such as Binder cumulant or spin stiffness the convergence of the scaling to infinite sizes will be more rapid (Beach et al., 2005; Ran et al., 2019). Our purpose is to extract the best estimates of g_c and ν from the (Q)MC data. For this aim, we expand a size-independent singular quantity Q , for which case $\kappa = 0$, to a Taylor series to the first order about the critical point,

$$Q(\delta, L) \approx a_0 + b_1 \delta L^{1/\nu} + c_1 L^{-\omega} \quad (1.21)$$

where the value of the λ is suppressed in the constant c_1 . The curves of Q in the vicinity of g_c intersect for different values of L . The crossing points of the couples (L, rL) systematically shift towards the g_c by increasing L for a constant $r > 1$. Thus a series of crossing point analyses can be conducted systematically starting from the Eq. (1.21).

Let $\delta^* = g_L - g_c$ be the value of the control parameter at the intersection of size

couples (L, rL) . Thus we can write $Q(\delta^*, L) = Q(\delta^*, rL)$ and if we solve for δ^* we find,

$$g_L - g_c \propto L^{-1/\nu-\omega} \quad (1.22)$$

where all the coefficients coming from r and Taylor expansion are combined. The value of g_c can then be estimated by making a curve fitting to Eq. (1.22) using a (Q)MC data with good statistics. The determination of the values of g_L is also another interpolation problem near g_c such that a fine grid of points each generated from a large number of MCS is required. We can estimate the value of $1/\nu$ by using the values of the derivatives of $Q(\delta, L)$ at g_c such that,

$$Q'(0, L) = \frac{dQ(0, L)}{d\delta} = bL^{1/\nu} \quad (1.23)$$

which can be linearized and the slope gives the value of $1/\nu$,

$$\ln Q'(0, L) = \tilde{b}_1 + \frac{1}{\nu} \ln L. \quad (1.24)$$

Eq. (1.24) requires relatively larger system sizes for a reliable fit and the value of g_c should be estimated before. Alternatively by including the second-order terms in the Taylor series of the scaling function a direct estimator of the correlation length exponent can be deduced,

$$Q(\delta, L) \approx a_0 + b_1\delta L^{1/\nu} + c_1L^{-\omega} + a_2\delta^2 L^{2/\nu} + b_2L^{-2\omega} + c_2\delta L^{1/\nu-\omega} \quad (1.25)$$

We now take the derivative of Eq. (1.25) at the point δ^* (at $\delta = 0$ the derivative still leads to Eq. 1.24) and after rearranging the constants the following is found,

$$Q'(\delta^*, L) = b_1 L^{1/\nu} (1 + \tilde{c}_2 L^{-\omega}). \quad (1.26)$$

from which $1/\nu$ can be left out as a fit parameter by taking the logarithm of the ratio of $Q'(\delta^*, rL)$ and $Q'(\delta^*, L)$, and the leading term of L^{-w} is kept

$$\frac{1}{\ln r} \ln \frac{Q'(\delta^*, rL)}{Q'(\delta^*, L)} = \frac{1}{\nu} + aL^{-w} \quad (1.27)$$

where a is a constant. Both methods for estimating ν will be tested.

1.2.3 Disorder Effects

Real systems are inevitably impure either accidentally or intentionally. The effect of random disorder on zero and finite temperature properties is one of the basic problems in condensed-matter physics. Randomness on a system might have different effects such as suppressing the critical temperature, destroying an ordered state, or even preserving the order with a different universality class. Statistically, the disorder can be handled as either annealed or quenched in which the disorder is included in the partition function as an additional degree of freedom for the former and the positions of the disorder are fixed to predefined values for the latter. Although the annealed disorder is easier to deal with analytically, the purpose of QMC methods is to overcome the infinite dimensionality of the partition function. On the other hand, it is not necessary to obtain infinitely many disorder realizations for the quenched averages. The self-averaging property of random systems makes it convenient to work with quenched disorder numerically (Aharony et al., 1998; M. Vojta, 2003; Wiseman & Domany, 1998).

For the lattice models, the disorder can lie on the sites or bonds of the system. According to the desired distribution, in the site disordered systems, magnetic ions are substituted by different species and in the bond disorder case, the interaction strengths are replaced. At what extent does the introduced disorder affect a system? The disorder can be treated as a crossover phenomenon from the pure case in the RG language. If one can quantify the considered disorder as an RG variable then it can be searched near the critical point of the pure system whether the disorder exponent is relevant or not. Here the relevancy is not the change in the critical temperature but is another universality class. For the simplest case, the weak disorder, the heuristic argument is due to Harris and has also been worked out in the frame of RG led to the following criterion (Hertz, 1985; T. Vojta & Sknepnek, 2004):

$$d\nu > 2. \quad (1.28)$$

The Harris criterion is the condition of the stability against a weak disorder of the pure system or in other words, it is the condition of irrelevance in RG sense. Recent theoretical studies and simulations try to classify the disorder systems in a unified manner such as

making connections between the Harris criterion and quantum Griffiths singularities
(T. Vojta & Hoyos, 2014).



CHAPTER TWO

QUANTUM MONTE CARLO METHODS

Computational physics is an intermediate discipline and it is on a way to be a separate branch at the undergraduate level. Among all the computational techniques the one dominates the field is the MC methods due to the same origin with statistical physics. One commonality of all MC methods is the random numbers. Thanks to the modern high-level programming languages we don't need to care about the desired quality of (pseudo) random numbers except for a particular reason. Any MC based approach that is used to try to solve a quantum mechanical problem is a QMC method. A QMC method in principle is generally nothing than any (classical) MC technique that is used to solve the Ising model. Most QMC methods use the Metropolis algorithm as their core. As the preceding chapter gives the clue, a QMC approach in d dimensions is mapped to a $(d + 1)$ -dimensional classical problem via the Feynman path integral. So the understanding of MC methods that are suited to solve classical statistical mechanics problems such as the Ising model is crucial. The classical representation of our analytical and numerical techniques seems to be inevitable in the present time that our computers are still classical so as our mathematics! The other classical representation is the high-temperature Taylor series expansion of the quantum partition function. This is the basis of the modern SSE QMC method.

Giving a fully pedagogical background of QMC techniques is beyond the contents of a dissertation. MC methods in statistical physics is a prerequisite up to some context and given in excellent books (Krauth, 2006; Landau & Binder, 2014; Newman & Barkema, 1999). Nevertheless, the important concepts such as the Metropolis algorithm, ergodicity, local, and global detailed balance should be mentioned.

2.1 Monte Carlo for Classical Spin Systems

The starting point for a statistical mechanical problem is the partition function of the system. The expectation value of a quantity A is an average over all the states

$\{\mu \mid \mu \in \{\mu_1, \mu_2, \dots\}\}$ of the system with Boltzmann probability,

$$\langle A \rangle = \frac{\sum_{\mu} A e^{-\beta E_{\mu}}}{\sum_{\mu} e^{-\beta E_{\mu}}}. \quad (2.1)$$

Here β is the inverse temperature with unit Boltzmann constant and E_{μ} is the energy of the system in the μ th state. There are infinitely many states μ for a large enough physical system. It is not possible to count all the states numerically and get physical averages. Actually the real physical system visits a very small portion of all the microstates during equilibrium even they appear in the partition function. The underlying concept of MC in statistical physics is to pick up these *important* states in a clever way which is called importance sampling. As a numerical method, this is an MC integration which is suitable for high-dimensional integrals.

The most clever choice of important states is to sample them with Boltzmann probability such that the Eq. (2.1) reduces to a simple estimator (Newman & Barkema, 1999). If we pick up M states this estimator is given by,

$$A_M = \frac{1}{M} \sum_i^M A_{\mu_i} \quad (2.2)$$

and for $M \rightarrow \infty$, $A_M = \langle A \rangle$. The problem is not fully covered yet. Although the procedure up to this point fits the logic of the MC, choosing the important states is not so easy. This problem has been overcome by constructing a Markov process which is common almost in all MC schemes. With a well-defined transition probability $W(\mu_j \rightarrow \mu_{j+1})$ the process $\mu_1 \rightarrow \mu_2 \rightarrow \dots \rightarrow \mu_M$ will tend to or *equilibrate* to Boltzmann distribution for a large enough M (Binder & Heermann, 2019). The transition between any two states depends only on these two states, not any others. After a sufficient number (M) of generated states, the fluctuations of a quantity can be monitored by directly averaging with Eq. (2.2).

One question remains on how to define the transition probability (W) between the states. First of all, in the course of a Markov process, a finite transition probability is expected from a selected state to any of the all possible states including itself. This is the

principle of *ergodicity*. It is important to realize that the transition probability from a state μ to ν in a single step can safely be set to zero but the state ν should be accessible through a Markov process. The other important point is the principle of *detailed balance*. It is based on the fact that in equilibrium¹ the transition rates to and from a state μ are intuitively expected to be equal. On the statistical grounds, the transition probability can be considered as a conditional probability i.e. the probability of being in state ν given the probability of being in state μ or vice versa:

$$W(\mu \rightarrow \nu) = P(\nu|\mu) \quad (2.3)$$

The rest is surprisingly to apply the Bayes' rule,

$$P(\mu)P(\nu|\mu) = P(\nu)P(\mu|\nu) \quad (2.4)$$

or equivalently,

$$P(\mu)W(\mu \rightarrow \nu) = P(\nu)W(\nu \rightarrow \mu). \quad (2.5)$$

There are a number of schemes that satisfy the principle of detailed balance and ergodicity such as Metropolis and heat bath algorithms.

The Metropolis algorithm is the most important and the first one being proposed. In the Metropolis algorithm the transition probability is factorized into selection (or proposition) $g(\mu \rightarrow \nu)$ and acceptance probabilities $A(\mu \rightarrow \nu)$ (Gubernatis et al., 2016; Newman & Barkema, 1999). In a system with N spins the selection probabilities are $g(\mu \rightarrow \nu) = 1/N$ and cancel out each other in Eq. (2.5). Thus the relative probabilities of transition and acceptance are equal:

$$\frac{A(\mu \rightarrow \nu)}{A(\nu \rightarrow \mu)} = \frac{P(\nu)}{P(\mu)}. \quad (2.6)$$

With the choice of Boltzman probability $P(\mu) \sim e^{-\beta E_\mu}$, the Metropolis algorithm is given in its simplest form by the acceptance probability,

$$A(\mu \rightarrow \nu) = \min\{1, e^{-\beta(E_\nu - E_\mu)}\}. \quad (2.7)$$

¹We don't touch to the master equation concept that deals with the time rate change of the transition probabilities which is zero in equilibrium but it is very important for completeness.

Proposing and deciding whether or not to flip spins N times according to Eq. (2.7) is called a single MC sweep (MCS) and it is equivalent to N MC steps per site. It is clear that one MCS is the unit time of the simulation. As one can guess something should be paid for this clever process. The consecutive configurations in the Markov chain are highly correlated. Only the configurations which are separated by some number of MCS are independent. A careful statistical analysis is needed for the calculation of quantities of interest.

The key property that makes the Metropolis algorithm so efficient is that a proposal from a higher energy state to lower one is always accepted. No algorithm is the most efficient one. Especially the MC algorithms can feel the critical slowing down of a phase transition. Many algorithms have been devised to overcome the drawbacks of the others. For example, the Wolff cluster flipping algorithm works very well in the vicinity of a phase transition in the Ising systems. This brief introduction to the Metropolis algorithm is thought to suffice for a background to the SSE QMC method.

2.2 Monte Carlo for Quantum Spin Systems

For spin models that include quantum effects, the MC simulations at finite temperatures can be exhibited by two main schemes the PIMC and the SSE QMC methods as mentioned in the preceding chapter. Both of these schemes *classicize* the quantum problem and are based on the quantum partition function of the bosonic lattice Hamiltonian. In quantum statistical mechanics the thermal average of a quantity is given by

$$\langle A \rangle = \frac{1}{\mathcal{Z}} \text{tr} \left(A e^{-\beta \mathcal{H}} \right) \quad (2.8)$$

where $\mathcal{Z}$ is the quantum partition function of the system. In the PIMC formalism, the exponential operator of the partition function is decomposed as a product of time slice operators:

$$e^{-\beta \mathcal{H}} = \prod_i^L e^{-\Delta \tau \mathcal{H}}, \quad (2.9)$$

where $\Delta \tau = \beta/L$. The equivalence between the exponential operator and the Schrödinger time evolution operator enables one to define the imaginary time $it = \Delta \tau$. In general the

Hamiltonian consists of non-commuting parts such as kinetic and potential terms. While the time-discretized algorithms rely on the Trotter-Suzuki approximation, the modern continuous-time PIMC techniques eliminate the decomposition error at the algorithmic level. In the SSE QMC formalism, the exponential operator is series expanded:

$$e^{-\beta\mathcal{H}} = \sum_n \frac{(-\beta)^n}{n!} \mathcal{H}^n. \quad (2.10)$$

This series converges with a finite number of terms for a finite temperature. The main advantage of this convergence is that as a discretized method it gives results with negligible errors in contrast to the imaginary-time discretization of the PIMC method that requires extrapolation to the continuous imaginary time at the algorithmic level.

Both formalisms are extended by choosing a complete set of states and inserting *closure* relations between every occurrence of the local operators that compose the Hamiltonian $\mathcal{H}$. Historically these formulations have been simulated by local updates (Hatano & Suzuki, 1993; Sandvik, 1992; Sandvik & Kurkijärvi, 1991) that have many drawbacks such as critical slowing down and non-ergodicity. Although the SSE and the continuous-time PIMC techniques give exact results with local updates they still exhibit critical slowing down and can not change the temporal and spatial winding numbers with a reasonable probability. As in the case of classical algorithms, cluster updating has been developed for quantum systems. The loop algorithm (Evertz, 2003) and its continuous-time variant (Beard & Wiese, 1996) have been the first and still widely used cluster updates in the framework of the PIMC method. The standard loop algorithm can be very inefficient for some problems such as Heisenberg antiferromagnet with a uniform strong magnetic field. For applicability to a more general class of models, the loop concept has been generalized to the worm algorithm (Kawashima & Harada, 2004; Prokof'ev et al., 1998).

On the SSE QMC side, although the loop concept can be applied to the series expansion representation (Evertz, 2003) as a cluster updating scheme, Sandvik (1999) developed the more efficient operator-loop update which is a worm-like algorithm. The importance of this method as mentioned above is that it has a discretized representation with loop cluster updates and gives exact results within the error bars without the need for

any extrapolation. Again for the applicability to the more general class of models more efficiently Syljuåsen and Sandvik (2002) developed another worm-like updating scheme the so-called directed-loop algorithm not only for the series expansion representation but also for the PIMC framework. The word *directed* indicates predefined probabilities for the worm head e.g. minimizing the backtracking probability. In the limit of zero-field, the directed-loop algorithm is continuously equivalent to the operator-loop algorithm i.e. it does not suffer algorithmic discontinuity. The SSE QMC with operator-loops and directed-loops has been used increasingly due to its efficiency for quantum spin systems and convenient and versatile implementation².

The operator-loop algorithm can successfully simulate the XXZ-model with external magnetic fields but the directed-loop algorithm is more efficient and equivalent to the operator-loop algorithm in the absence of fields. As a starting point of an MC method for quantum spin systems, the operator-loop SSE QMC method can well be preferred. In the following sections, we give formalism and diagonal updating mechanism of the general SSE QMC method. The operator-loop algorithm is given for the specific spin-1/2 isotropic Heisenberg (XXX) model.

2.2.1 SSE Formalism

The quantum partition function is written as a Taylor series expansion with a chosen basis and closure relations as follows,

$$\mathcal{Z} = \text{tr} \left(e^{-\beta \mathcal{H}} \right) = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}} \langle \alpha_0 | \mathcal{H} | \alpha_{n-1} \rangle \cdots \langle \alpha_2 | \mathcal{H} | \alpha_1 \rangle \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle \quad (2.11)$$

where $\{\alpha\} = \alpha_0, \alpha_1$, etc. and the indices of α can be related to imaginary time. As a general property, by using the Eq. (2.8) with $A = \mathcal{H}$, a simple relation for the total internal energy can be derived:

$$E = \frac{1}{\mathcal{Z}} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}} \langle \alpha_0 | \mathcal{H} | \alpha_n \rangle \cdots \langle \alpha_2 | \mathcal{H} | \alpha_1 \rangle \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle \quad (2.12)$$

²Andres W. Sandvik has been awarded the 2021 Aneesur Rahman Prize for Computational Physics Recipient “for the development of the stochastic series expansion algorithm, and for numerous creative applications of this method to the study of quantum phase transitions.”

Here, after making the substitution $n \rightarrow n - 1$, the series can still start from $n = 0$,

$$E = \frac{1}{\mathcal{Z}} \sum_{n=0} \frac{(-\beta)^n}{n!} \frac{n}{-\beta} \sum_{\{\alpha\}} \langle \alpha_0 | \mathcal{H} | \alpha_{n-1} \rangle \cdots \langle \alpha_2 | \mathcal{H} | \alpha_1 \rangle \langle \alpha_1 | \mathcal{H} | \alpha_0 \rangle \quad (2.13)$$

that matches the right-hand side of the Eq. (2.11) apart from a constant which gives the energy estimator as,

$$\langle \mathcal{H} \rangle = E = -\frac{\langle n \rangle}{\beta}. \quad (2.14)$$

Thus the internal energy can simply be calculated by monitoring the fluctuations of the number of operators in the simulations. Many quantities have simple estimators in terms of the number of operators in the SSE formalism for which more formal derivations will be given in the following sections.

The Hamiltonian $\mathcal{H}$ consists of the sum of local operators such as Eq. (1.12) for a lattice system. Local terms of the Hamiltonian generally include two-body operators and single-site terms and can be written in terms of the bonds that are two interacting sites. Namely, the Hamiltonian of a system with N sites and N_b bonds can be decomposed as follows,

$$\mathcal{H} = \sum_{i,j}^N H_{i,j} = - \sum_b^{N_b} H_{i(b),j(b)} = - \sum_b^{N_b} H_b \quad (2.15)$$

where the minus sign convention removes the sign problem explicitly in the exponential operator and the single-site terms should include correct compensation due to the over-summing e.g., the uniform fields $h_i = h$ should be scaled with the factor $\delta = N_b/N$ such that $h_{i(b)} = h_b \sim h/\delta$. For a Hamiltonian on a d -dimensional cubic lattice with NN interactions and uniform external field the scaling factor is $\delta = d$. An implicit negative sign in the products of the local operators is still present that will be clear in the following sections and can be removed for a variety of important systems. Insomuch that the diagonal part of the local operator can always be made positive by a suitable constant but the negative sign stemming from the off-diagonal part is avoided under special circumstances such as in an antiferromagnetic system on a bipartite lattice.

The next step in the formulation of the SSE technique is to substitute the sum over bonds into the Eq. (2.11). After one realizes that the *products of sums* can be written as

the *sums of products*, the quantum partition function includes the form of sums over bond indexes:

$$\mathcal{Z} = \sum_{n=0} \frac{\beta^n}{n!} \sum_{\{\alpha\}} \sum_{\{b\}} \langle \alpha_0 | H_{b_n} | \alpha_{n-1} \rangle \cdots \langle \alpha_2 | H_{b_2} | \alpha_1 \rangle \langle \alpha_1 | H_{b_1} | \alpha_0 \rangle \quad (2.16)$$

where $\{b\} = b_1, b_2, \text{etc.}$ and each $b_i = 1, 2, \dots, N_b$. This formalism is somewhat similar to the Eq. (2.9) with inserted closure relations between time slice operators and then traced out. Of course, the Eq. (2.16) can be written without closure relations in a compact fashion,

$$\mathcal{Z} = \sum_{n=0} \frac{\beta^n}{n!} \sum_{\alpha} \sum_{\{b\}} \left\langle \alpha \left| \prod_i^n H_{b_i} \right| \alpha \right\rangle, \quad (2.17)$$

here any propagated state is expected to be proportional to another single basis state. This no-branching condition is satisfied by splitting the local bond operator to further parts such as diagonal and off-diagonal. For example, if one splits the local operator into two parts there will be $M = 2N_b$ possible H_b with $b = 1, 2, \dots, M$. A double index such as $H_{a,b}$ where $a = 1, 2, \dots$ and $b = 1, 2, \dots, N_b$ be the operator type and the bond number, respectively, might make the formalism more readable and in the next sections, these conventions will be used interchangeably but for computer implementation, a 1D array is more convenient. We treat here any operator H_b with this no-branching property and write the p -th propagated state,

$$|\alpha(p)\rangle \propto \prod_i^p H_{b_i} |\alpha(0)\rangle \quad (2.18)$$

where $|\alpha(0)\rangle = |\alpha\rangle$ and for $p = n$ we must have $|\alpha(n)\rangle = |\alpha(0)\rangle$ due to the periodicity. What is sampled in Eq. (2.17) is the state $|\alpha\rangle$ and the operator sequence (or string) $S_n = H_{b_n} \cdots H_{b_2} H_{b_1}$ and they constitute a *configuration* (α, S_n) . Thus the basic mechanism of the SSE QMC method is to sample the configurations,

$$(\alpha, S_n) = \langle \alpha | S_n | \alpha \rangle = \langle \alpha | H_{b_n} \cdots H_{b_2} H_{b_1} | \alpha \rangle \quad (2.19)$$

to find the terms that have significant contributions to the quantum partition function. Most of the configurations give zero contribution to the partition function so only the allowed ones should be attempted. This restriction makes a QMC algorithm very

efficient with a cleverly devised algorithm. In other words, one does not need to cover all configuration space as in the classical spin models but a very restricted portion of it. We now write the weight function,

$$\mathcal{W}(\alpha, S_n) = \frac{\beta^n}{n!} \langle \alpha | H_{b_n} \cdots H_{b_2} H_{b_1} | \alpha \rangle = \frac{\beta^n}{n!} \left\langle \alpha \left| \prod_i^n H_{b_i} \right| \alpha \right\rangle \quad (2.20)$$

which is to be positive definite. The weight can be made positive definite by properly splitting the local operator as mentioned above. If can't, the simulations still can be carried out with positive and negative weights by using $|\mathcal{W}|$ which will produce uncontrollable errors when approaching larger system sizes and lower temperatures. This is a definition of the notorious sign problem.

The convergence property of the SSE can be used for a more efficient updating of the operator string and easier implementation (Sandvik, 1997). The series expansion can be truncated after several terms, $n_{\max} = L$, which are sufficient for the convergence and exponentially small negligible error. This representation is called the fixed-length scheme which will transform the explicit summation over n to an implicit one. For the cut-off $n_{\max} = L$ the series Eq. (2.17) is written as follows,

$$\mathcal{Z} = \sum_{\alpha} \left\langle \alpha \left| 1 + \beta \sum_{b_1} H_{b_1} + \frac{\beta^2}{2!} \sum_{b_1, b_2} H_{b_1} H_{b_2} + \cdots + \frac{\beta^L}{L!} \sum_{\{b\}} H_{b_1} H_{b_2} \cdots H_{b_L} \right| \alpha \right\rangle \quad (2.21)$$

where one should notice that the empty product, the term corresponding to $n = 0$, is equal to 1. There is nothing new in this expansion. The last term already contains L operator products or in other words, it is the operator string with length L . The purpose is to make all the operator strings with length L that can be accomplished by inserting a sufficient number of *unit* operators. A unit operator $I = H_0$ does not affect the result of any operator string wherever it is placed. All the operator strings contain n non-unit operators and need $L - n$ unit operators to complete their length to L . The total number of ways that an operator string with length n can be completed to the string with fixed-length L by using the unit operators is exactly equal to the binomial coefficient $\binom{L}{n}$. One should pay for an extra term for each index b_i to keep the length of the string fixed,

and should compensate each term with $\binom{L}{n}$. Namely, we should realize the following:

$$\sum_{n=0}^L \sum_{b_1, b_2, \dots, b_n} H_{b_1} H_{b_2} \cdots H_{b_n} = \frac{n!(L-n)!}{L!} \sum_{b_1, b_2, \dots, b_L} H_{b_1} H_{b_2} \cdots H_{b_L} \quad (2.22)$$

where $b_i = 1, 2, \dots, M$ on the left side and $b_i = 0, 1, \dots, M$ on the right side. Thus if we extend the indices of the last (the longest string) term of Eq. (2.21) to include $b_i = 0$ it will over-sum the terms $n \leq L$ implicitly. The final form of the SSE formalism for a Hamiltonian with a total of M pieces of local operators on a lattice with any geometry is given as in the following:

$$\mathcal{Z} = \sum_{\{\alpha\}} \sum_{\{b\}} \frac{\beta^n (L-n)!}{L!} \langle \alpha_0 | H_{b_L} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | H_{b_2} | \alpha_1 \rangle \langle \alpha_1 | H_{b_1} | \alpha_0 \rangle \quad (2.23)$$

where n is then the number of non-unit operators in the string, i.e., the number of operators H_b with $b \neq 0$ and the indices $b_i = 0, 1, \dots, M$. What is the optimal value of L ? A very high value of L e.g. 10^6 will mostly work fine to get negligible errors or exact results but it wastes CPU. The internal energy per spin is given by $E/N = -\langle n \rangle / N\beta$ according to Eq. (2.14) which shows that L scales as βN . The optimal value of L can be determined self-consistently throughout the equilibration of a simulation that will be explained later in this chapter.

We did not touch on the QMC methods for ground-state calculations. Both methods PIMC and SSE can technically be used for ground-state calculations. Because the SSE method is a high-temperature series expansion, for big values of β and site number N the operator string length L will become very high that might require hundreds of hours of CPU time for a single simulation. The modern algorithms for the ground-state simulations that are variants of PIMC and SSE formalisms with minor modifications include variational and projector QMC methods (Sandvik & Evertz, 2010). Although the computational effort is drastically reduced with the projector and variational simulations the SSE QMC method can be used in a robust way to reach the ground-state properties due to the availability of the high-performance computing (HPC) centers which can supply hundreds of CPU resources at a time and the simulations can be run in an embarrassingly parallel manner not just for $T = 0$ calculations but also for finite temperatures. Besides,

there are tricks for efficient ground-state convergence such as β -doubling procedures (Peng et al., 2020; Sandvik, 2002a). As a final remark for this section, the PIMC and SSE formalisms are equivalent for limits $\Delta\tau \rightarrow 0$ and $L \rightarrow \infty$, respectively, in which they have the same weight β^n/L^n (Sandvik, 2019). The fundamental difference between the PIMC and SSE techniques is that while the former is exact after the limit, the latter is exact already before the limit, i.e. for a finite L .

Dynamical quantum calculations in real-time which are important as well as difficult to compute and are out of our scope in this study. In the next section, the diagonal updating is detailed based on the general formalism of the SSE QMC method and the detailed balance concept of the Metropolis acceptance probabilities.

2.2.2 Diagonal Updates

In the SSE method, the local bond operators are of type either diagonal and/or off-diagonal. In the fixed-length scheme of the SSE formalism there is an extra unit operator. There are N_b possible locations on the lattice for each operator type. The number of operator types is depended on the model interested. For example, in the double index notation $H_{a,b}$, the type indexes can take values $a = 1, 2$ and $a = 1, 2, 3$ for the $S = 1/2$ and $S > 1/2$ 1D Heisenberg models, respectively (Sandvik & Kurkijärvi, 1991). There are examples of four and eight different local bond operator types in the simulations of Hubbard and spin-Peierls models (Sandvik, 1992; Sandvik et al., 1994; Sandvik et al., 1997).

There are two basic updating schemes in the SSE method, diagonal and loop (operator or directed) (Sandvik, 1999; Syljuåsen & Sandvik, 2002). The diagonal update replaces a unit operator with a diagonal operator and vice versa. Remembering that we did not put any restriction on the Hamiltonian in the Eq. (1.9) until now the diagonal update is applicable to the general spin- S systems (Henelius et al., 2002). The bond operators can be labeled arbitrarily and for convenience we define the operators H_b with $1 \leq b \leq N_b$ (the first N_b odd or even numbers can be set for a convenient computer implementation as we do in the next section) as the diagonal operators. First we rewrite the weight function

Eq. (2.20) by using the Eq. (2.23) of the fixed-length operator sequence formalism,

$$\mathcal{W}(\alpha_0, S_L) = \frac{\beta^n (L - n)!}{L!} \langle \alpha_0 | H_{b_L} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | H_{b_2} | \alpha_1 \rangle \langle \alpha_1 | H_{b_1} | \alpha_0 \rangle. \quad (2.24)$$

Here if any of the elements $\langle \alpha_p | H_{b_p} | \alpha_{p-1} \rangle$ vanishes the weight $\mathcal{W}(\alpha_0, S_L)$ is not allowed and should not be produced in an updating (diagonal or loop) procedure. Diagonal and unit operators do not change the state to which they act on. But diagonal operators can give zero (or they are arranged so not just for a convenient and efficient implementation but also for positive definiteness) when acting on specific states. This means that updating from a diagonal operator to a unit operator is always allowed but the reverse is not. In an actual simulation, in the diagonal updating procedure, the diagonal and unit operators in the string $H_{b_1} H_{b_2} \cdots H_{b_L}$ are traversed sequentially and if the proposed operator gives an allowed configuration it is accepted with the Metropolis probability that satisfies the detailed balance equation, i.e., the Eq. (2.5). For an efficient implementation, only one of the states $|\alpha_p\rangle$ is stored in the computer's memory and the stored state is propagated according to the visited operator type while traversing the operator string.

In a diagonal updating, only the operator string S_L changes so we can define the convention for the transition $(\alpha, S_L) \rightarrow (\alpha, S'_L) = (S_L \rightarrow S'_L)$. For a single update the number of non-unit operators n in the operator string changes as $n \rightarrow n \pm 1$. The probability of a configuration (α_0, S_L) is proportional to $\mathcal{W}(\alpha_0, S_L)$. Now we write the detailed balance equation,

$$\mathcal{W}(\alpha_0, S_L) A(S_L \rightarrow S'_L) g(S_L \rightarrow S'_L) = \mathcal{W}(\alpha_0, S'_L) A(S'_L \rightarrow S_L) g(S'_L \rightarrow S_L) \quad (2.25)$$

where

$$\mathcal{W}(\alpha_0, S'_L) = \frac{\beta^{n \pm 1} (L - (n \pm 1))!}{L!} \langle \alpha_0 | S'_L | \alpha_0 \rangle \quad (2.26)$$

for a single updating procedure in which the string S'_L departs from S_L with a single diagonal bond operator, and we can define $(H_0 \rightarrow H_b)$ for the plus sign and $(H_b \rightarrow H_0)$ for the minus sign. There are N_b choices from a unit to a diagonal operator transition thus for the selection probability we have $g(H_0 \rightarrow H_b) = 1/N_b$ but for the reverse, i.e. from a diagonal to a unit operator, there is only one choice and $g(H_b \rightarrow H_0) = 1$. In an

attempt to update an operator H_{b_p} the element $\langle \alpha_p | H_b | \alpha_{p-1} \rangle$ with $1 \leq b \leq N_b$ will survive on one side of the Eq. (2.25). Because the diagonal and unit operators do not affect the states, here we have $|\alpha_p\rangle = |\alpha_{p-1}\rangle$. With these at hand, we write the following,

$$\frac{\mathcal{W}(\alpha, S'_L)}{\mathcal{W}(\alpha, S_L)} = \frac{(L - (n \pm 1))!}{(L - n)!} (\beta \langle \alpha_p | H_b | \alpha_p \rangle)^{\pm 1} \quad (2.27)$$

and the rest is to write the Metropolis acceptance probabilities

$$A(H_0 \rightarrow H_b) = \min \left[1, \frac{N_b \beta \langle \alpha_p | H_b | \alpha_p \rangle}{L - n} \right] \quad (2.28a)$$

$$A(H_b \rightarrow H_0) = \min \left[1, \frac{L - n + 1}{N_b \beta \langle \alpha_p | H_b | \alpha_p \rangle} \right]. \quad (2.28b)$$

The acceptance probabilities might take different forms depending on the system for example in models with arbitrary interactions (Sandvik, 2003). The second type of update is between the diagonal and off-diagonal operators. The local off-diagonal updates are not ergodic, e.g. they can not change the winding number. So extra updating types are required such as ring updates (Sandvik et al., 1997). As mentioned before, the operator and directed loop algorithms together with the diagonal updating make the simulation nearly or fully ergodic (Sandvik, 1999; Syljuåsen & Sandvik, 2002). In the following section, we give an application to the spin-half AFM Heisenberg model in one and two dimensions which is a good starting point for the understanding of the implementation of the SSE QMC method with operator-loops before extending it to a more general class of models. Besides, notions of the general algorithm will also be touched on for foreknowledge when an emphasis is considered.

2.2.3 SSE for Spin-1/2 Heisenberg Model

Here we first write the Eq. (2.15) or equivalently the Eq. (1.12) with $\Delta = 1$ (isotropic) and $h_i = 0$ in terms of bonds by preserving the sign convention,

$$\mathcal{H} = \sum_b^{N_b} J_b \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)} = - \sum_b^{N_b} H_b \quad (2.29)$$

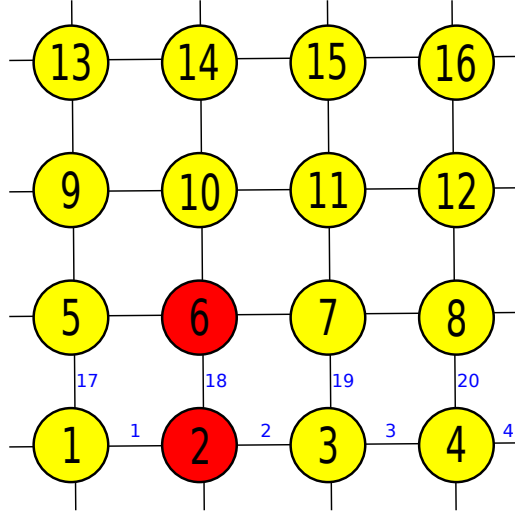


Figure 2.1 Schematic representation of NN site bonds on a 2D square lattice with periodic boundary conditions. The bonds are labeled first from left to right and then from bottom to top. This labeling is arbitrary and there are $2 \times 16 = 32$ bonds in total. As an example, the 18th bond connects the sites $i(18) = 2$ and $j(18) = 6$

which can technically describe a wide range of models where J_b is the coupling constant at bond b and $S_{i(b)}$ are spin operators at sites $i(b)$. A schematic representation of the relation between the bond and site numbers is shown in Figure (2.1) on a 2D square lattice with periodic boundary conditions. There are $N = 16$ sites on the lattice and for the NN interactions, there are $N_b = 32$ bonds. The bonds are labeled first left to right and then bottom to top as shown with the numbers between the sites in the figure. As an example, the bond $b = 18$ connects the sites $i = 2$ and $j = 6$, thus $i(18) = 2$ and $j(18) = 6$. The bonds can be constructed arbitrarily. If the site numbers are defined with the bonds for the interested model, no further modifications needed for the rest of the SSE code except for the corresponding bond strengths J_b .

The only restriction to the implementation procedures that will be explained in this section is the spin value which is $S = 1/2$ here. The subsequent implementation steps can be applied to the (quantum) spin systems with $S = 1/2$ that can be described by Eq. (2.29) in any geometry and dimension. Of course, the sign problem may appear in frustrated geometries or interactions. So the applied systems are selected with the interactions either ferromagnetic ($J_b < 0$) or antiferromagnetic ($J_b > 0$) on a bipartite lattice in which a NN site is always on the opposite sublattice. It is worth stressing that the values of J_b can be selected from any desired distribution which property extends

the range of problems to disorder systems. In the next chapters, the explained procedures in this section will be applied to disorder systems with important physical properties.

The local operator H_b is divided into two pieces $H_{1,b}$ and $H_{2,b}$,

$$H_{1,b} = \frac{1}{4} \pm S_{i(b)}^z S_{j(b)}^z \quad (2.30a)$$

where the plus and minus signs stand for ferromagnetic and antiferromagnetic interactions, respectively and

$$H_{2,b} = \frac{1}{2} \left(S_{i(b)}^+ S_{j(b)}^- + S_{i(b)}^- S_{j(b)}^+ \right), \quad (2.30b)$$

here $H_{a,b}$ is the diagonal and off-diagonal operator for $a = 1, 2$ respectively. Thus for those models we have $M = 2N_b$ local operators. The Hamiltonian is then rewritten in terms of the local bond operators $H_{a,b}$ as follow,

$$\mathcal{H} = - \sum_b^{N_b} |J_b| (H_{1,b} \pm H_{2,b}) + \sum_b^{N_b} \frac{|J_b|}{4} \quad (2.31)$$

in which the second sum is a constant and will be omitted in the formulations and simulations, but it can be added to internal energy as a shift if desired in the post-simulation procedures. We now write the SSE formalism in the fixed-length scheme using the double index notation for the aforementioned model,

$$\mathcal{Z} = \sum_{\alpha} \sum_{\{a\}, \{b\}} \frac{\beta^n (L-n)!}{L!} \left\langle \alpha \left| \prod_p^L |J_{b_p}| H_{a_p, b_p} \right| \alpha \right\rangle \quad (2.32)$$

where $a_p = 1, 2$, and $b_p = 1, 2, \dots, N_b$ and $(a_p, b_p) = (0, 0)$ corresponds to the unit operator $H_{0,0}$. First, we write the matrix elements of $H_{a,b}$ which is an operator of connected two sites that requires the basis set $\{|\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle\}$. There are sixteen matrix elements for each operator type and only two of them are non-zero. The diagonal operator has the following non-zero matrix elements for the ferromagnetic case,

$$\langle \downarrow\downarrow | H_{1,b} | \downarrow\downarrow \rangle = \langle \uparrow\uparrow | H_{1,b} | \uparrow\uparrow \rangle = \frac{1}{2} \quad (2.33a)$$

and for the antiferromagnetic case

$$\langle \downarrow \uparrow | H_{1,b} | \downarrow \uparrow \rangle = \langle \uparrow \downarrow | H_{1,b} | \uparrow \downarrow \rangle = \frac{1}{2} \quad (2.33b)$$

and the off-diagonal operator has the following non-zero matrix elements,

$$\langle \downarrow \uparrow | H_{2,b} | \uparrow \downarrow \rangle = \langle \uparrow \downarrow | H_{2,b} | \downarrow \uparrow \rangle = \frac{1}{2} \quad (2.33c)$$

The equality of these matrix elements assure a convenient implementation of the SSE method as well as positive definiteness. This is why the diagonal operators are shifted. Thus the weight of a configuration (α, S_L) is simply given by

$$\mathcal{W}(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!} \prod_{p=0}^{L-1} J_{b(p)} \quad (2.34)$$

and the Metropolis acceptance probabilities take a more compact form,

$$A(H_0 \rightarrow H_b) = \min \left[1, \frac{J_b N_b \beta}{2(L-n)} \right] \quad (2.35a)$$

$$A(H_b \rightarrow H_0) = \min \left[1, \frac{2(L-n+1)}{J_b N_b \beta} \right]. \quad (2.35b)$$

In the following, we give an example of an allowed configuration for the antiferromagnetic case and the propagation (from right to left) of the state, that will be used through the section to make the understanding of the method more concrete.

$$\begin{aligned} & \langle \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow | H_{1,6} H_{1,1} H_{2,7} H_{0,0} H_{2,3} H_{1,2} H_{0,0} H_{1,1} H_{2,7} H_{1,3} H_{0,0} H_{2,3} | \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \rangle \\ &= \frac{1}{2} \langle \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow | H_{1,6} H_{1,1} H_{2,7} H_{0,0} H_{2,3} H_{1,2} H_{0,0} H_{1,1} H_{2,7} H_{1,3} H_{0,0} | \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \rangle \\ &= \frac{1}{2} \langle \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow | H_{1,6} H_{1,1} H_{2,7} H_{0,0} H_{2,3} H_{1,2} H_{0,0} H_{1,1} H_{2,7} H_{1,3} | \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \rangle \\ &= \left(\frac{1}{2}\right)^2 \langle \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow | H_{1,6} H_{1,1} H_{2,7} H_{0,0} H_{2,3} H_{1,2} H_{0,0} H_{1,1} H_{2,7} | \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \rangle \\ &= \left(\frac{1}{2}\right)^3 \langle \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow | H_{1,6} H_{1,1} H_{2,7} H_{0,0} H_{2,3} H_{1,2} H_{0,0} H_{1,1} | \downarrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \rangle \\ &\quad \vdots \end{aligned}$$



Figure 2.2 Schematic representation of the allowed matrix elements. Each configuration is called a vertex. The striped and empty bars indicate diagonal operators for the ferromagnetic and antiferromagnetic cases, respectively. The filled bar shows the off-diagonal operator. Although the operator types are apparent from the states of the vertices they are indicated for clarity

$$= \left(\frac{1}{2}\right)^9.$$

The configuration is in one dimension with periodic boundary conditions and has $N = 8$ sites. The bonds are from left to right and $N_b = 8$, the length of the operator string is $L = 12$ with $n = 9$ non-unit operators. Thus the weight of the configuration is $\mathcal{W} = (\beta/2)^9 (12 - 9)! / 12!$. The off-diagonal operators appear in pairs on the same bond as can be seen from the example configuration ($H_{2,3}$ and $H_{2,7}$) otherwise neither the configuration is allowed nor it has a positive weight. Of course, the most trivial configuration is the one with all the operators are unit which is always allowed regardless of the states. At the start of a simulation, this property ensures an allowed configuration that composes of completely a random state and a string with all operators are unit, namely, $\langle \alpha | H_{0,0} H_{0,0} \cdots H_{0,0} | \alpha \rangle$.

The pictorial representation of the example configuration will make sense due to the similarity with the Euclidean path integral world-lines in continuous time (Syljuåsen & Sandvik, 2002). The allowed matrix elements given in Eq. (2.33) can be pictorially represented with four spin states and a compatible operator between the spin couples. Each representation for matrix elements is called a vertex and they are shown in Figure 2.2 for the ferromagnetic and antiferromagnetic cases.

It is easy to distinguish which operator type is used but for clarity, they are indicated with different drawings. The diagonal operators are indicated with striped and empty bars for the ferromagnetic and antiferromagnetic cases, respectively. The filled bar shows the off-diagonal operator and there is no need for a representation for the unit operators. Thus there are four vertices for each case. If the diagonal operators have not been shifted there would be six vertices for both cases but in the XXZ model with an external field, the number of vertices is six inevitably. We now sketch the example

p	$a(p)$	$b(p)$	$s(p)$	$v_0(p)$	v'	$v_1(p)$	v'	$v_2(p)$	v'	$v_3(p)$	v'
11	1	6	12	44	46	45	38	46	44	47	12
10	1	1	2	40	18	41	26	42	16	43	17
9	2	7	15	36	14	37	15	38	45	39	13
8	0	0	0	—	—	—	—	—	—	—	—
7	2	3	7	28	27	29	11	30	0	31	1
6	1	2	4	24	19	25	10	26	41	27	28
5	0	0	0	—	—	—	—	—	—	—	—
4	1	1	2	16	42	17	43	18	40	19	24
3	2	7	15	12	47	13	39	14	36	15	37
2	1	3	6	8	2	9	3	10	25	11	29
1	0	0	0	—	—	—	—	—	—	—	—
0	2	3	7	0	30	1	31	2	8	3	9

Figure 2.3 Extended configuration of the example configuration with the full propagated states for the antiferromagnetic case. The adjacent columns are the data structures that can be implemented with the appropriate programming utilities such as arrays and pointers. $v_l(p)$ is linked to the v' , and vice versa, i.e. $\text{link}(v_l(p)) = v'$ and $\text{link}[\text{link}(v_l(p))] = v_l(p)$

configuration with propagated states using the vertices. A configuration with propagated states is called the *extended* configuration. Examples of extended configurations are shown in Figure 2.3 and Figure 2.4 for the ferromagnetic and antiferromagnetic cases, respectively, by explicitly representing the *full* propagated states. The columns on the right side of the extended configuration show an example data structure that can be implemented on a computer.

The propagation index p is akin to the imaginary time concept of the PIMC method so it can be treated as the time dimension of the SSE method. $a(p)$ and $b(p)$ are the operator type and bond indices (from left to right), respectively, as before. In the fourth column, $s(p) = 2b(p) + a(p) - 1$ reduces the double index storage to a 1D array which can be used to reproduce either the operator type or the bond number, and $s(p) = 0$ corresponds to the unit operator. The extended configuration is not needed to be stored, instead, the required propagated configuration can be generated whenever an off-diagonal operator encountered while traversing the operator sequence in an updating process. Actually, the representation of all the propagated states is redundant. Only using the vertices an extended configuration can be depicted more abstractly as shown in Figure 2.5 and Figure 2.6 in which the consecutive extended configurations

p	$a(p)$	$b(p)$	$s(p)$	$v_0(p)$	v'	$v_1(p)$	v'	$v_2(p)$	v'	$v_3(p)$	v'
11	1	6	12	44	34	45	35	46	32	47	8
10	0	0	0	—	—	—	—	—	—	—	—
9	2	1	3	36	14	37	26	38	12	39	13
8	1	6	12	32	46	33	10	34	44	35	45
7	2	3	7	28	27	29	3	30	0	31	1
6	1	2	4	24	15	25	2	26	37	27	28
5	0	0	0	—	—	—	—	—	—	—	—
4	0	0	0	—	—	—	—	—	—	—	—
3	2	1	3	12	38	13	39	14	36	15	24
2	1	7	14	8	47	9	11	10	33	11	9
1	0	0	0	—	—	—	—	—	—	—	—
0	2	3	7	0	30	1	31	2	25	3	29

Figure 2.4 Extended configuration example with full propagated states for the ferromagnetic case. The adjacent columns are the data structures that can be implemented with the appropriate programming utilities such as arrays and pointers. $v_l(p)$ is linked to the v' , and vice versa, i.e. $\text{link}(v_l(p)) = v'$ and $\text{link}[\text{link}(v_l(p))] = v_l(p)$

differ by a single diagonal update from each other. For example, the third and the fourth configurations are connected via the updating $H_{0,0} \leftrightarrow H_{1,4}$ at the location $p = 8$ (or via $s(8) = 0 \leftrightarrow s(8) = 8$) in the Figure 2.5. Similarly, the third and the fourth configurations are connected via the updating $H_{0,0} \leftrightarrow H_{1,4}$ at the location $p = 4$ (or via $s(4) = 0 \leftrightarrow s(4) = 8$) in the Figure 2.6.

Here the value of p is only used as the argument of an array till now and has nothing to do as a variable. The p dependence of the vertices is needed for a random access to the position of each single spin site in the extended configuration space. For an efficient operator loop update procedure, a *linked* storage of the positions that connect the legs of the vertices on the same site in the extended configuration is needed. For this purpose, the legs of the vertices are labeled as $l = 0, 1, 2, 3$ starting from a reference leg (the left bottom leg here) and each leg position is assigned to the value $v_l(p) = 4p + l$. This will produce unique numbers for each position because there is only one operator for each value of p . As an example in the first extended configuration of Figure 2.5, the third leg ($l = 2$) of the vertex for $p = 2$ ($v_2(2) = 10$) is linked to the second leg ($l = 1$) of the vertex for $p = 6$ ($v_1(6) = 25$). Thus two elements of the linked-list can be defined as $\text{link}(10) = 25$ and $\text{link}(25) = 10$. For any two connected legs v and v' the list

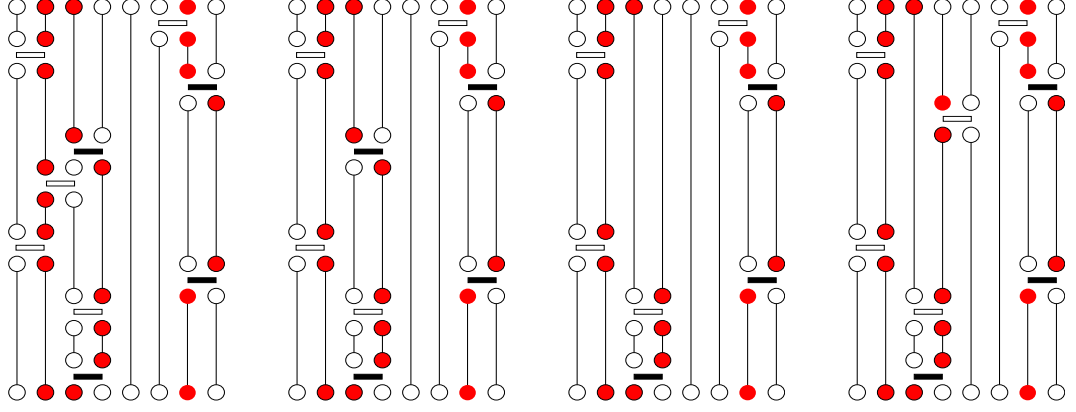


Figure 2.5 Description of an extended configuration in terms of allowed vertices of antiferromagnetic case. This is an abstract representation and the operator types are indicated explicitly for clarity as mentioned before. The consecutive configurations differ by a single diagonal update from each other, e.g., the first and the second configurations are connected by the updating $H_{1,2} \leftrightarrow H_{0,0}$ at the location $p = 6$ (or by $s(6) = 4 \leftrightarrow s(6) = 0$)

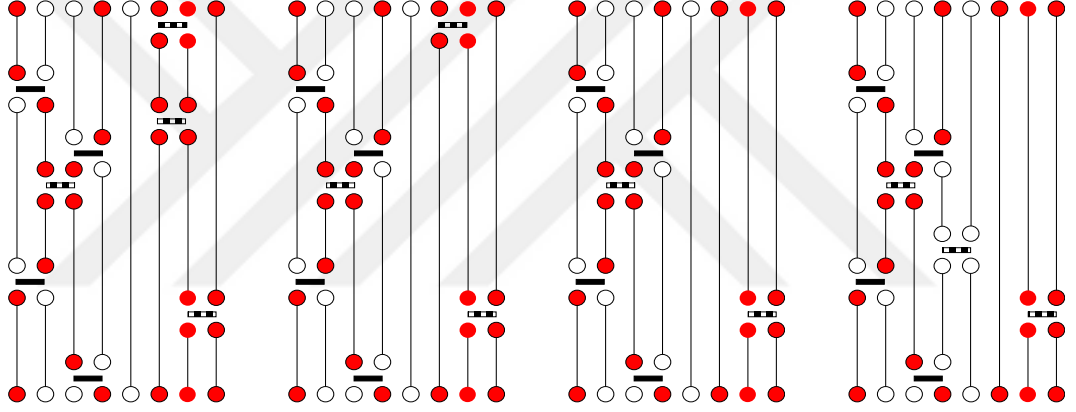


Figure 2.6 Description of an extended configuration in terms of allowed vertices of ferromagnetic case. This is an abstract representation and the operator types are indicated explicitly for clarity as mentioned before. The consecutive configurations differ by a single diagonal update from each other, e.g., the first and the second configurations are connected by the updating $H_{1,2} \leftrightarrow H_{0,0}$ at the location $p = 4$ (or by $s(4) = 4 \leftrightarrow s(4) = 0$)

contains the elements $\text{link}(v) = v'$ and $\text{link}(v') = v$. A full list is given in Figure 2.3 for the example configuration. It should be realized from the example linked-list that the legs are connected periodically across $p = 0$.

By using the linked-list we can *walk* on the extended configuration and construct a *loop*. The inter-vertex movement is ensured with the linked-list. What about an intra-vertex movement? Intuitively we see that inside a vertex we can go from a leg to another leg including itself. The examples for each possible intra-vertex move type are

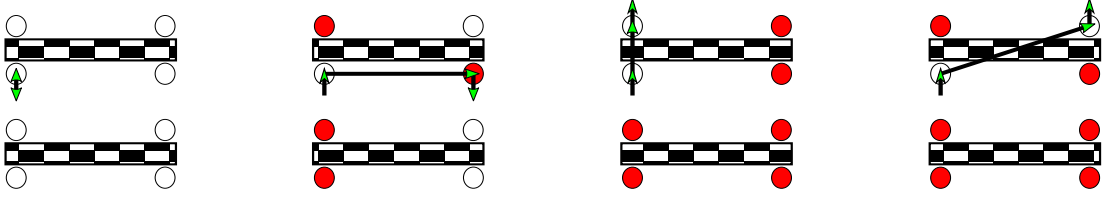


Figure 2.7 The examples of each intra-vertex movement with the first leg ($l = 0$) as the reference entrance leg. The resulting vertices after the spin flipping are shown below the examples. The bar with the checkerboard pattern is any type of operator

shown in Figure 2.7 with the first leg as the reference entrance. Any leg could be the entrance. We will call the move types to *bounce*, *switch*, *straight*, and *cross* as with the same order in Figure 2.7.

Thus there are four choices for the intra-vertex move and only one choice for the inter-vertex move. Inter- and intra-vertex movements follow each other until the loop closes. The loop will close when the starting leg is reached. Flipping the spins on the loop path *might* result in a new allowed configuration. If the problem were the general XXZ model with an external field this arbitrary loop constructing and flipping procedure would produce an allowed configuration with a higher probability compared to the model interested in here, i.e., the XXX model. As a result, this would be a very inefficient updating procedure for both models. As stated before, the aim is to propose updates (loops here) that produce allowed configurations. Instead, the loops can be constructed in a way provided that the resulting vertex is one of the allowed vertices after flipping the spins on the path in an intra-vertex move. Only the spins that the intra-vertex movement visits are flipped. No spins are flipped in an inter-vertex move. The bounce process visits the entrance leg twice so the net change is no spin flip and thus the bounce process is always allowed for any model. We did not tell anything about the operators in the loop constructing procedure. As mentioned before a vertex can completely be defined with its four spin states thus after the loop is constructed and the spins flipped the operators can easily be assigned to the new four spin states for each vertex.

For the model interested here, the spin-1/2 XXX model without external field, the permitted intra-vertex move types are very restricted and this is an advantageous for an efficient simulation of the model. For the antiferromagnetic (ferromagnetic) case,

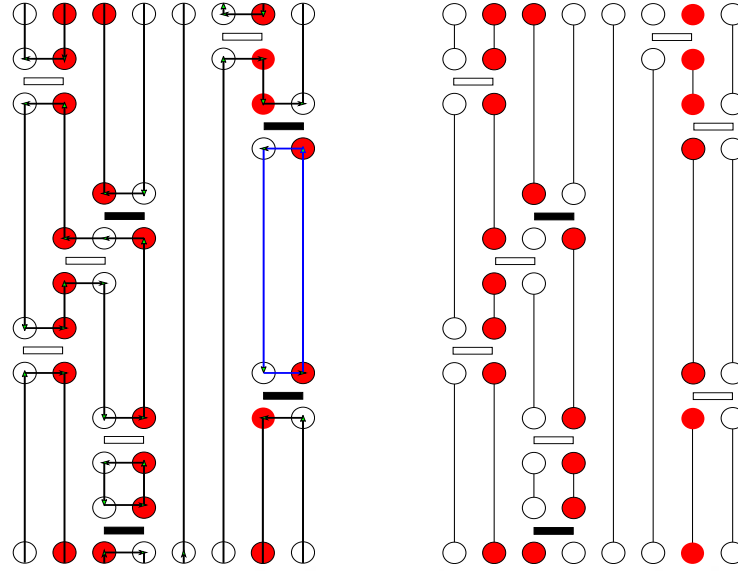


Figure 2.8 Example of loop update for the antiferromagnetic case. All the available loops are indicated on the left. The spins on a single loop are flipped and the corresponding operators are interchanged on the right. Loop paths that pass two sides of the vertex interchange the operator twice so it does not change but the spins on the vertex are flipped

only the *bounce* and the *switch* (*cross*) processes can generate allowed vertices. In other words, the loops that can give a new allowed configuration when the spins flipped on it are constructed by using only two intra-vertex movements at most for those models. Furthermore, the bounce process will not make an opportunity for a different loop because the only remaining possibilities are switch (*cross*) or another bounce for the antiferromagnetic (ferromagnetic) case. As a result, the only effect of the bounce movement is to slow down the loop construction process and it can be excluded for both cases. An example loop updating for the antiferromagnetic case is shown in Figure 2.8 in which all the loops are indicated on the left configuration and the spins on the path of a single loop are flipped on the right configuration.

The operators on the path also interchanged between the diagonal and off-diagonal. Different loop paths that passes two sides of the vertex interchange the operator twice so the operator does not change but the spins are flipped on the vertex. An example of loop updating for the ferromagnetic case is shown in Figure 2.9 and similar arguments follow. Spins in the extended configuration which do not belong to any vertex are called free spins and can be regarded as loops as shown in Figure 2.8 and Figure 2.9.

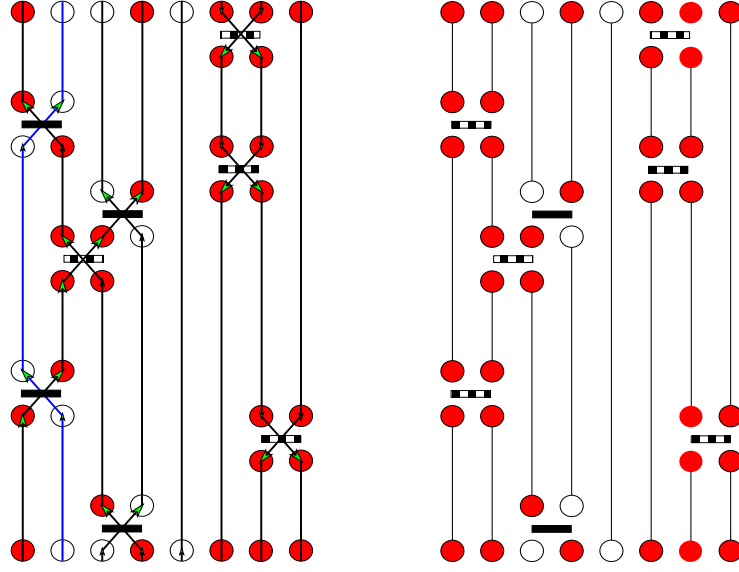


Figure 2.9 Example of loop update for the ferromagnetic case. All the available loops are indicated on the left. The spins on a single loop are flipped and the corresponding operators are interchanged on the right. Loop paths that pass two diagonals of the vertex interchange the operator twice so the operator type does not change but the spins on the vertex are flipped

We note here this is not the case for the general XXZ model in which the bounce process is not excluded and has a non-zero probability. The direction of the move can either be selected with heat-bath probabilities or with the probabilities determined by solving the directed loop equations which try to minimize the bounce probability. But for the cases handled here, there is no need to assign any probability to the direction of the intra-vertex movement because there is always only one direction which makes the loop construction *deterministic* and specifically, this procedure is called deterministic operator-loop update. In fact, for the fixed positions of the operators, the extended configuration can be break up into loops in a unique way. One question remains is that at what rate should the loops be flipped. Any flipping (or acceptance) probability will satisfy the detailed balance because the selection (proposed deterministically) probability is *one* and flipping the spins on a loop interchanges the corresponding operators between diagonal and off-diagonal only, i.e., the number of non-unit operators n does not change so the weight $\mathcal{W}(\alpha, S_L)$. In the original article, Henelius and Sandvik (2000) chose that probability to be 1/2 to flip or not the spins on the loop path.

Basically, a full traversing of the operator sequence for a diagonal update and flipping the spins on the path of each possible loop with a chance of one half on the extended

configuration is an MCS of the operator loop algorithm. The next section will include the algorithms with their pseudocode and other technical details such as the determination of the cut-off value for the length of the operator string.

2.3 Implementation Details

Trying to implement an algorithm whether with pseudocode or not is the most essential part of understanding the underlying logic of a numerical method. In this section, we give the pseudocodes of the implementation of the deterministic operator-loop algorithm for the isotropic $S = 1/2$ Heisenberg model with $|J_b| = 1$. The diagonal update followed by the loop update constitutes one MCS of the simulation so they are the heart of the algorithm and repeated on average hundreds of thousands of times. It will be convenient to keep the configuration (α, S_L) as separate integer 1D arrays, namely `state(j)` and `string(p) = s(p)`, respectively. As mentioned earlier, the most trivial configuration is a random spin state and an operator string with all operators are unit. It can be generated easily as an initial configuration. Before going into details we give some details of hardware and compiler properties for the reproducibility of the results given here. A GNU Fortran compiler with version 9.3.0 on an Intel(R) Core(TM) i5-4300U CPU is used. The intrinsic Fortran function `random_number` with seed value 17684860 and seed size 12 is used to generate pseudorandom numbers in the interval $[0, 1)$. Systems in one and two dimensions with 16 spins are used with NN interactions and periodic boundary conditions in all dimensions for the test results. The initial configuration (both in one and two dimensions) is produced with the random state, `state = [1 -1 -1 1 -1 -1 1 -1 1 1 1 -1 -1 -1 1 1]` and operator sequence of length 4, `string = [0 0 0 0]`. The bonds are constructed at the initialization of the simulation and which is intended to be the only change for different dimensions and geometries. The hierarchy of Figure 2.1 is used for bonds and a 2D array of size $2 \times N_b$, `bond`, is declared for storing the labels that connect all NN sites periodically, e.g., `bond[1, 21] = 5`, `bond[2, 21] = 9`, `bond[1, 32] = 16`, `bond[2, 32] = 4`. Other variables are the same as in the text otherwise stated such as `p` for propagation index, `n` for the number of non-unit operators, etc and some of them will be deducible in the pseudocode. The pseudocode of the diagonal update is given in Figure 2.10 which cares about all the possibilities when inserting a

```

1: for p = 0 to L - 1 do
2:   op ← string(p)
3:   if op = 0 then
4:     b ← random(1, 2, ..., Nb)
5:     if state(bond(1, b)) = ±state(bond(2, b)) then
6:       P01 ←  $\frac{N_b \beta}{2(L-n)}$ 
7:       r ← random_number
8:       if r < P01 then
9:         string(p) ← 2b
10:        n ← n + 1
11:       end if
12:     end if
13:   else if op mod 2 = 0 then
14:     r ← random_number
15:     P10 ←  $\frac{2(L-n+1)}{N_b \beta}$ 
16:     if r < P10 then
17:       string(p) ← 0
18:       n ← n - 1
19:     end if
20:   else
21:     b ← op/2
22:     state(bond(:, b)) ← -state(bond(:, b))
23:   end if
24: end for

```

Figure 2.10 The pseudocode for diagonal update

diagonal operator. The plus and minus signs in the Line 5 correspond to the ferromagnetic and antiferromagnetic cases, respectively. The only constraint on removing a diagonal operator is the acceptance probability.

The number n fluctuates in the diagonal update block of the simulation code and can be averaged outside of the block to compute the relevant quantities such as the internal energy in Eq.(2.14). Other important estimators such as specific heat, staggered susceptibility can be written compactly depended on n and they will be given in a separate section. The variables P01 and P10 correspond to the Eq. (2.35a) and Eq. (2.35b), respectively. The statement in Line 21 is an integer division.

Provided that the linked-list of the labels of legs in the extended configuration is constructed, the loops can be created by starting from the first leg of the first non-unit

operator in the imaginary time direction. Technically to achieve this the links should include extra information. There are $4L$ legs in an extended configuration but $4n$ of them are visible on a graph. The rest belongs to unit operators and can be linked to a constant number such as minus one that distinguishes them from the others, i.e. $\text{link}(v_1(p)) = -1$ for all $s(p) = 0$. The first occurrence of a leg along the imaginary time dimension is kept to track the free spins, i.e., the sites with no operator on it, as well as to connect the legs across the time boundary. It is stored in an array called `first` separately and assigned to a minus number at the beginning of the construction of a linked-list. If no leg is connected to any vertex the corresponding array element will not change during the linked-list construction and the minus number will indicate a free spin for that site. The non-zero element of the array `first` is used to connect the last leg along the same direction across the time boundary periodically. For example, the fifth site of the example configurations of both ferromagnetic and the antiferromagnetic cases have no leg that is connected to any vertex, i.e., $\text{first}(5) = -1$.

Due to the deterministic nature of the loops for the present models, the entrance legs can be attempted in sequential order. We remember the labeling of a vertex here: $l = 0, 1, 2, 3$ for the bottom left, bottom right, top left, and top right legs of a vertex, respectively. Actually, for any arbitrary labeling, the exit leg can be determined for all types of intra-vertex movements practically by using bit intrinsic logical operations. For all purposes, a bitwise exclusive-OR (`xOR`) operation does the job. It can be defined as $\text{xOR}(l_e, m) = l_x$ in which l_e and l_x are the entrance and the exit legs, respectively, and the integer m chooses the type of the intra-vertex movement. In our labeling of vertex legs, $m = 1$ and $m = 3$ correspond to the switch and cross types of moves for the antiferromagnetic and ferromagnetic cases, respectively. It is clear that for a model that includes non-deterministic loops the value of m can be selected randomly among the leg numbers, which is the case for the more general heat-bath or directed loop algorithms. High-level programming languages incorporate bit intrinsic procedures for machine-independent logical operations e.g., the bitwise operators `ieor` and `^` (caret symbol) are available for the Fortran and C/C++ programming languages, respectively. These bitwise operators can be used for any entrance leg $l_e = v_1(p) = 4p + 1$.

In the construction of all loops, it is enough to traverse only half of the total number of legs. Because when a leg is selected the next leg is definite in an intra-vertex move. Thus, for both ferromagnetic and antiferromagnetic cases, looping over either even or odd integers will suffice. As said before arbitrary labeling of the legs of vertices is possible. For example, the labeling $l = 0, 2, 3, 1$ with $m = 1$ and $m = 3$ ensures the desired looping procedures for the ferromagnetic and antiferromagnetic cases, respectively. But as another example, the labeling $l = 0, 3, 1, 2$ with $m = 2$ (ferromagnetic) and $m = 3$ (antiferromagnetic) requires something different looping variables to traverse the half of the legs for an efficient calculation.

The first step is to test whether the leg belongs to any vertex or to a unit operator. If it belongs to a vertex then the entrance leg is stored in another variable to close the loop later. A random number is generated before the loop construction. The flipping of the spins on the loop may be rejected but the loop is constructed anyway to not construct it over again. The construction firstly starts with an intra-vertex movement and continues until the loop closes, i.e., the entrance and exit legs meet. For accepted loops the operator sequence is updated immediately with the virtue of xOR operation. After all the available loops are constructed the spins are flipped on the accepted ones. As mentioned previously only one state is stored and the spin states in the extended configuration is not stored in the memory. It is important to realize that only the accepted loops that cross the time boundary at $p = 0$ can cause a change in the state of the configuration. To achieve this the first links of each site is assigned to minus one for rejected loops and minus two for accepted loops. Thus after constructed all loops the array `link(first(i))` can either be minus one or minus two for all `first(i) ≥ 0` and the sites for all `first(i) < 0` correspond to free spins as mentioned before. The pseudocode for the full process of the loop algorithm is given in Figure 2.11 that corresponds to ferromagnetic and antiferromagnetic cases for $m = 3$ and $m = 1$, respectively. The divisions in Line 8 are integer divisions.

This completes an MCS of the deterministic operator-loop algorithm of the SSE method for the isotropic spin-1/2 (anti)ferromagnetic model in any (unfrustrated) geometry and dimension.

```

1: for l = 0 to 2 × L - 1 do
2:   le ← 2 × l
3:   if link(le) ≠ -1 then
4:     lx = le
5:     r ← random_number
6:     if r < 1/2 then
7:       loop
8:         string(lx/4) = xOR(string(lx/4), 1)
9:         link(lx) = -2
10:        lt = xOR(lx, m)
11:        lx = link(lt)
12:        link(lt) = -2
13:        if lx = le then
14:          exit loop
15:        end if
16:      end loop
17:   else
18:     loop
19:       link(lx) = -1
20:       lt = xOR(lx, m)
21:       lx = link(lt)
22:       link(lt) = -1
23:       if lx = le then
24:         exit loop
25:       end if
26:     end loop
27:   end if
28: end if
29: end for
30: for i = 1 to N do
31:   if first(i) < 0 then
32:     r ← random_number
33:     if r < 1/2 then
34:       state(i) = -state(i)
35:     end if
36:   else if link(first(i)) = -2 then
37:     state(i) = -state(i)
38:   end if
39: end for

```

Figure 2.11 The pseudocode for loop update

The linked-list should be constructed after the diagonal update but before the operator loop update. The first step in the construction of the links is explained above with the role of the array `first`. The links are created for each site separately. For the rest of

the links, we need another array variable, say `last`. We can think of the `link(s)` of a single site for a better understanding. Suppose that the very first leg of the site `i` is at the `p`-th vertex. After assigning the variable `first(i)` to a minus integer the variable `last(i)` is assigned to the other leg in the same site, i.e., $\text{last}(i) = 4p + 2$. When the second or more times the site `i` is visited the value stored in the `last(i)` is linked to the selected new leg number. For this process, a temporary variable is needed. And to make the algorithm work the lists `first` and `last` must be updated for the sites `i` and `j` consecutively which are on the same bond for the selected vertex `p`. This is required because two legs that are linked to each other may be on different bonds. The construction procedure is more clear in the pseudocode that is given in Alg-4. The links are connected periodically using the values in the list `first` and the very last values in the list `last`. The lists `link`, `first`, and `last` are assigned to appropriate negative values such as minus one before every construction. Lines 4, 5, 6, and 7 are aligned (0, 1, 2, 3) to show the labeling part of the legs of the construction. The pseudocodes given up to now are written to make the algorithm more clear but during the coding, they can be made more efficient and changed structurally depending on the capabilities of the programming language or interpreter used, e.g., using extra temporary variables.

The heart of the SSE simulation is the diagonal, and operator loop updates together with the linked-list construction. A diagonal update followed by the construction of the linked-list, and loop update is the most time-consuming part of the simulation. The initialization process of the simulation includes the generation of a random configuration, the construction of bonds, and the determination of constants such as the temperature and size of the system. After the initialization, the system should be equilibrated to the desired conditions. At this part, the actual simulation is run for a few thousands of steps to drive the system from the random initial configuration to an instant of the equilibrated system. The spin states and the operator string (i.e., the configuration) are updated and the length (`L`) of the operator string, i.e., the truncation value of the series is determined self-consistently at this stage.

The length of the string does not have a definite value, the optimal length is the one that is just above the maximum number of non-unit operators. Because the number of non-unit

```

1: for p = 0 to L - 1 do
2:   b ← string(p)/2
3:   if b ≠ 0 then
4:     leg0 ← 4 × p + 0
5:     leg1 ← leg0 + 1
6:     leg2 ← leg0 + 2
7:     leg3 ← leg0 + 3
8:     i ← bond(1, b) ; j ← bond(2, b)
9:     legi ← last(i) ; legj ← last(j)
10:    if legi < 0 then
11:      first(i) ← leg0
12:    else
13:      link(legi) ← leg0
14:      link(leg0) ← legi
15:    end if
16:    last(i) ← leg2
17:    if legj < 0 then
18:      first(j) ← leg1
19:    else
20:      link(legj) ← leg1
21:      link(leg1) ← legj
22:    end if
23:    last(j) ← leg3
24:  end if
25: end for
26: for s = 0 to N do
27:   if first(s) ≠ -1 then
28:     link(last(s)) ← first(s)
29:     link(first(s)) ← last(s)
30:   end if
31: end for

```

Figure 2.12 The pseudocode for construction of the linked-list

operators is sampled thorough the simulation the length of the operator string should exceed the maximum of the number of non-unit operators. During the equilibration, the length of the operator string (L) is adjusted to a value which is determined by increasing the number of non-unit operators (n) by a predefined percentage (a) whenever the string length exceeds that value. The practical value of that percentage is between 30% and 50% (Sandvik, 2019). In this way, the value of L is kept at a small value for an efficient simulation and at a large enough value to sample n safely. The new value of L includes a copy of its previous content augmented by unit operators. The unit operators can be augmented at arbitrary positions in the last operator string, in any case, it will be a

valid configuration. For almost all purposes $a = 3$ is thought to be enough but it is safer to check the margin between the maximum of n and L before starting the measuring physical observables. The part of the pseudocode for updating the length of the operator string is given in Figure 2.13. The first line is an integer division. A temporary array

```

1:  $\Delta n \leftarrow n/a$ 
2: if  $n > L - \Delta n$  then
3:   allocate memory for string_copy(0 : L - 1)
4:   string_copy  $\leftarrow$  string
5:    $L_{\text{new}} \leftarrow n + \Delta n$ 
6:   deallocate memory of string
7:   allocate memory for string(0 : Lnew - 1)
8:   string(0 : L - 1)  $\leftarrow$  string_copy(0 : L - 1)
9:   deallocate memory for string_copy
10:  deallocate memory for link
11:   $L \leftarrow L_{\text{new}}$ 
12:  allocate memory for link(0 : 4 \times L - 1)
13: end if

```

Figure 2.13 The pseudocode for updating the string length

`string_copy` is required to augment unit operators to operator string. The arrays should be (de)allocated when necessary. In the Figure 2.13 the unit operators are augmented to the end of the `string` but they can freely be inserted at any location by using the capabilities of the programming language used, e.g., by using a random *mask*. The array `link` should also be reallocated when the `string` length changes.

A full simulation process is given in the Figure 2.14. Here the equilibration and the actual simulation processes are the same except for the part of updating the operator string length. Each consecutive diagonal update, linked-list construction, and loop update correspond to an MCS of the simulation. After each MCS the length of the operator string is updated if necessary in the first loop, and measurement of the physical observables are performed in the second loop. The construction of bonds is dependent on the geometry and the interaction of the interested system. Some examples of bond construction are given in the appendix for selected models.

```

1: declare all necessary variables and constants
2: allocate(string(0 : L - 1))
3: allocate(link(0 : 4 × L - 1))
4: create a random spin state
5: construct bonds
6: for i = 1 to mcs_cut do
7:     diagonal update
8:     construct linked-list
9:     loop update
10:    update string length
11: end for
12: for i = 1 to mcs do
13:     diagonal update
14:     construct linked-list
15:     loop update
16:     measure physical observables
17: end for
18: post simulation procedures

```

Figure 2.14 The full SSE QMC pseudocode for the spin-1/2 isotropic Heisenberg model

2.3.1 Simulation Details

In this section, we give some test results for the isotropic spin-1/2 (anti)ferromagnetic model with NN interactions and periodic boundary conditions in one and two dimensions. The system sizes are restricted to $N = 16$ for comparability with ED results. The equilibration process for the antiferromagnetic chain at $\beta = 100$ is shown in Figure 2.15. For all different values of a the expansion cut-off L is above the maximum of n at all intervals. We use $a = 3$ for all the subsequent computations hereafter.

The graph in Figure 2.15 is a time series for n and it is clear that the consecutive values are highly correlated. Measurements separated more than autocorrelation times are required for reliable statistics. Autocorrelation times are not much longer than a few MCS for the loop updates (Sandvik, 2010a). Instead, one can measure quantities at each MCS provided that the total number of MCS is much longer than the autocorrelation time. Each average by this procedure will be an independent measurement and distributed to a Gaussian which is guaranteed by the central limit theorem. The number of independent simulations depends on the model studied. For models that do not involve any kind

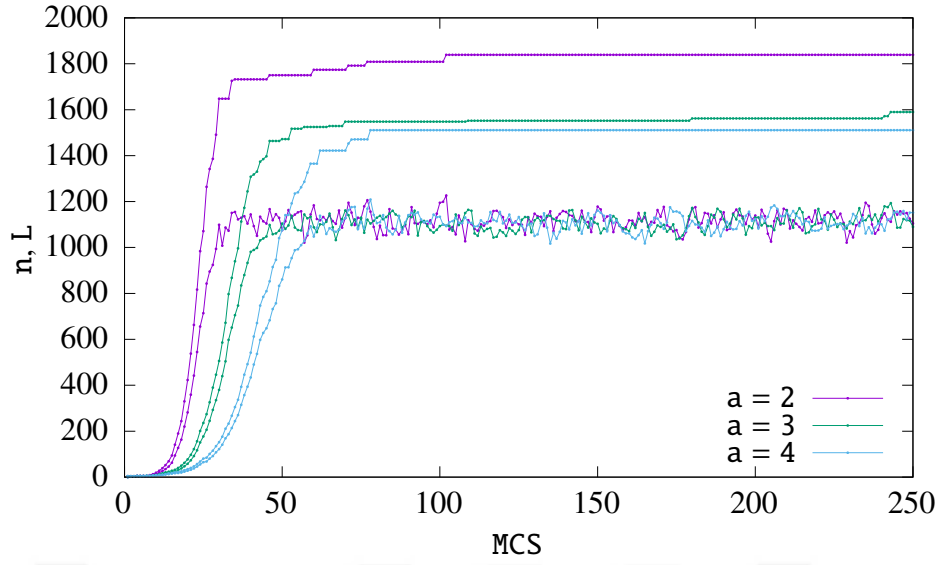


Figure 2.15 Equilibration process of a 1D chain with model parameters $N = 16$, $\beta = 100$, and $J_b = 1$ for different values of a

of random disorder, i.e., clean systems, independent measurements on the order of ten will be sufficient for most purposes. But for disordered systems, independent measurements on the order of hundreds to thousands might be necessary. For clean systems, the simulations can be performed in a single very long run then divided into several bins. Each bin average can be used as an independent measurement. Alternatively, the same copy of the simulation can be run several times long enough with different pseudo-random number seeds to get independent measurements. With statistically independent data at hand, one can make the error analysis of the measured quantities. For directly measured quantities standard error analysis is suitable. For derived quantities, the errors should be propagated. Generally, the standard error propagation suffices for the analysis of the derived quantities but some non-linear quantities such as Binder cumulant might require more advanced error analysis, e.g., Jackknife or bootstrap error propagation techniques.

In the disordered systems, the random disorder enters into the problem as an additional degree of freedom. Due to the self-averaging property of disorder systems one single simulation is enough for each realization. Thus the average of each realization can be used as a bin and the error analysis can be performed in the same way with the

clean system. The drawback for the disorder systems is that they require averages over hundreds or thousands of random realizations to get the correct statistics. This trouble can be overcome in an embarrassingly parallel manner with enough high-performance computing (HPC) resources that can provide calculations of thousands of realizations at once. The minimum number of realizations required can be determined by making a running average of a quantity near a critical point if present.

Some test results are given in Table 2.1 for the internal energy and the results are compared with the ED calculation of the quantum Heisenberg antiferromagnetic chain. The first line includes the result for a single run. The results are the same up to four decimal digits but the fourth digit is not reliable and might be a coincidence. The second and the third rows have quite correct results calculated from twenty and fifty independent simulations with the standard error given in the parentheses. The run time of the QMC calculation is a few seconds on a standard computer for each simulation. It is important to note here that the computation time for the ED calculation is on the order of ten hours.

Table 2.1 Test results for the internal energy and the comparison with the exact value for the quantum Heisenberg antiferromagnetic chain of length $N = 16$

#	β	MCS_CUT	MCS	$-E/N$ (QMC)	$-E/N$ (ED)
1				0.446346	
20	100	5×10^3	5×10^4	0.44640(3)	0.4463935
50				0.44640(2)	

Similar results are given in Table 2.2 for the ferromagnetic case. The QMC results are exact up to some precision for both cases. The accuracy and the precision of the results show the power of MC methods in general. The ground state energy of both models is exact for the given system size but only the result of the ferromagnetic case is the same as the one in the thermodynamic limit. The exact value of the ground state for the spin-1/2 isotropic antiferromagnetic Heisenberg chain in the thermodynamic limit can be calculated exactly using the Bethe Ansatz as $-E/N = \ln 2 - 1/4 = 0.443147$. The SSE method is a high-temperature series expansion method so it operates very efficiently at finite temperatures but it is also possible to make simulations in the ground state for any system size due to the powerful computational resources.

Table 2.2 Test results for the internal energy and the comparison with the exact value of the quantum Heisenberg ferromagnetic chain of length $N = 16$

#	β	MCS_CUT	MCS	$-E/N$ (QMC)	$-E/N$ (ED)
1				0.249955	
20	500	5×10^3	5×10^4	0.25001(2)	0.2500000
50				0.25000(1)	

SSE QMC results for the 1D and 2D isotropic Heisenberg model are given below for various quantities in which each average value is calculated from a 32 independent simulation run with the same MCS and MCS_CUT parameters of Table 2.1 and compared with ED calculation results. Total energies for both cases are given in Figure 2.16 where the energies are shifted by the constant in the Eq. (2.31) to meet the ED results. The results are exact for all cases so the error bars are not visible. The total energy is an off-diagonal observable and easily measured by monitoring the number of non-unit operators n .

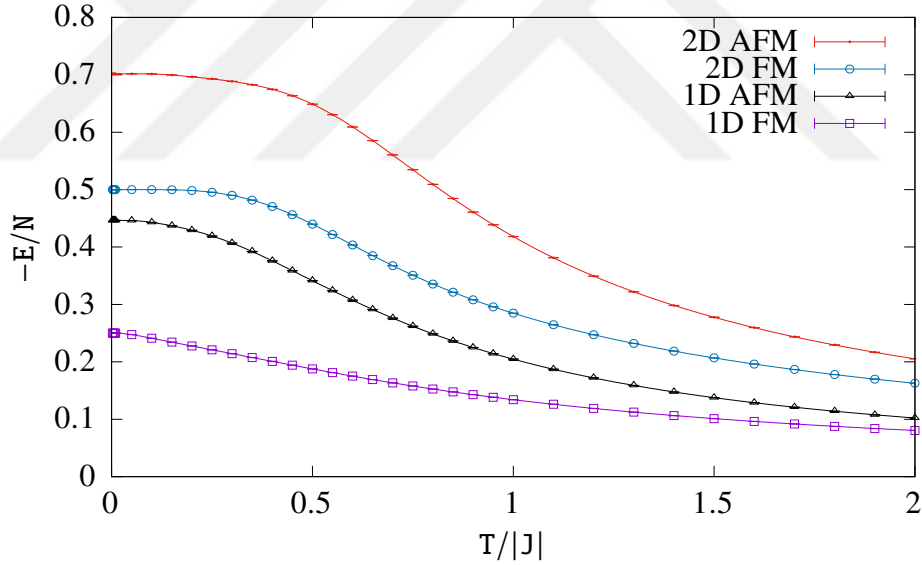


Figure 2.16 Energy per site results with SSE QMC and ED methods for comparison. The solid lines are ED results of a thousand temperature points

The heat capacity is also an off-diagonal operator and is measured with the following simple estimator:

$$C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle \quad (2.36)$$

which will be derived later. It is difficult to compute the specific heat at low temperatures

reliably because the number of non-unit operators is very high in this regime but the expected differences from Eq. (2.36) are tiny. The heat capacity per site values are compared with ED results as shown in Figure 2.17 and it can be seen that the errors get higher across the lower temperatures. The error bars are calculated by propagating the standard errors of the terms in Eq. (2.36) with the Jackknife technique. The constant that is present in the energy cancels out when calculating the specific heat so it is not needed as a post-simulation process.

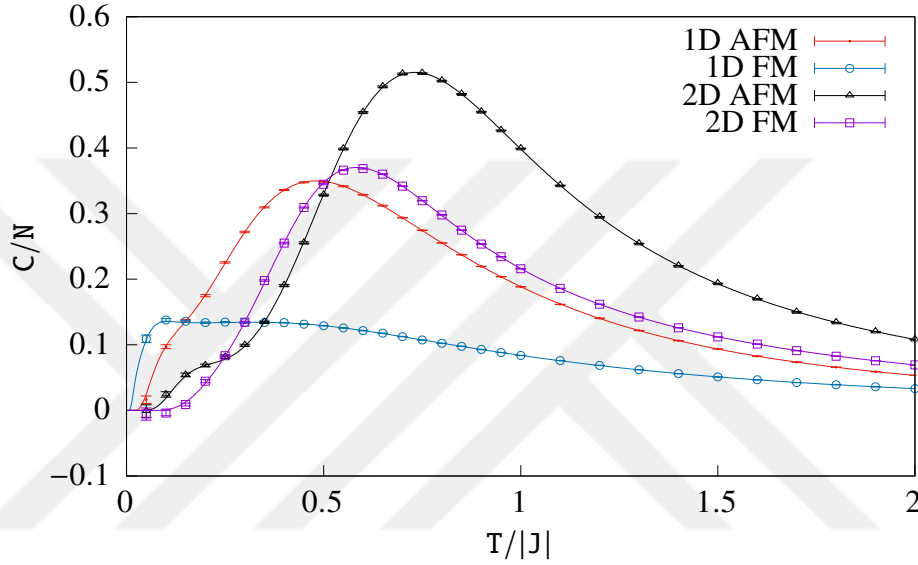


Figure 2.17 Specific heat per site results with SSE QMC and ED methods for comparison. The solid lines are ED results of a thousand temperature points

Diagonal observables are easier to calculate. z-component of the total spin operator can be measured and it is related to uniform magnetic susceptibility per site of the system via the relation:

$$\chi = \frac{\beta \langle (S^z)^2 \rangle}{N}. \quad (2.37)$$

The uniform magnetic susceptibility results are given for both the ferromagnetic and the antiferromagnetic cases separately in Figure 2.18 and Figure 2.19, respectively. All results fit well with the ED results and have very small error bars.

Another useful quantity is measured by monitoring the absolute value of S^z at each MCS. The results of $\langle |S^z| \rangle$ are shown in Figure 2.20 by comparing with ED calculations. The error bars are very small at all temperatures. Some operators such as the z-component

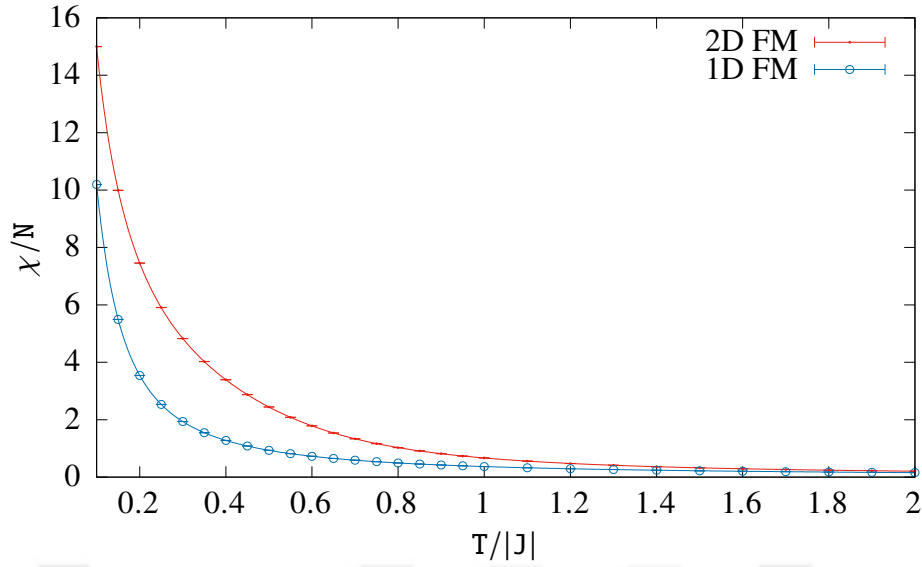


Figure 2.18 Uniform susceptibility per site results of the ferromagnetic case from SSE QMC and ED methods for comparison. The solid lines are ED results of a thousand temperature points

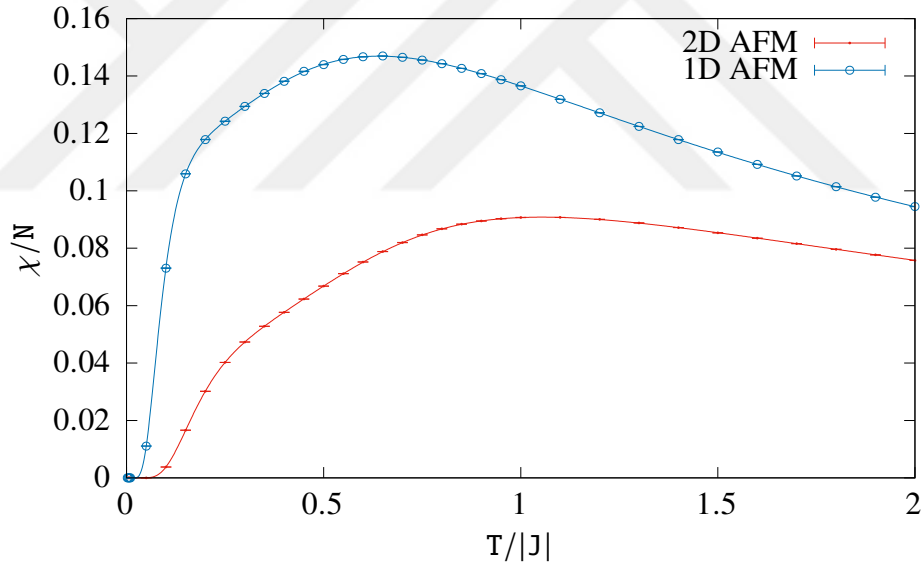


Figure 2.19 Uniform susceptibility per site results of the antiferromagnetic case from SSE QMC and ED methods for comparison. The solid lines are ED results of a thousand temperature points

of the squared staggered magnetization in Eq. (1.11) require an internal average over the full propagated states at each MCS. One can propagate the state as in Lines 21 and 22 of Figure 2.10 and accumulate the value of observable for all $p = 0, 1, \dots, L - 1$. Alternatively, the internal average can be performed over the extended configuration with no unit operators or at some steps to increase the speed. Traversing the whole

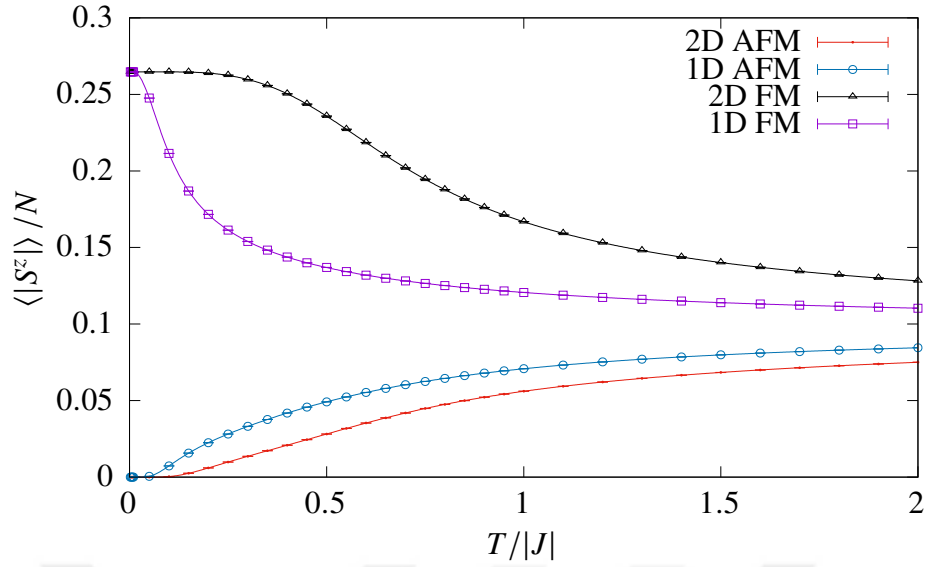


Figure 2.20 Absolute value of S^z per site results of the (anti)ferromagnetic case from SSE QMC and ED methods for comparison. The solid lines are ED results of a thousand temperature points

propagated states might consume time especially at low temperatures because it contains the same number of iterations as much as the case of diagonal update. It should be realized that the value of S^z does not change at any propagated state for the models interested here so it is not necessary to perform an internal average over propagated states for that quantity but the staggered magnetization changes due to the phase factor in its definition.

Squared staggered magnetization is an important quantity because it is related to the structure factor. The simulation results for other important quantities such as structure factor, staggered susceptibility, spin stiffness will be given for realistic models in the following chapters after we give a formal derivation of the estimators.

2.4 Estimators

Firstly, we rewrite some basic equations of the SSE formalism. The thermal expectation value of an operator,

$$\langle \mathcal{A} \rangle = \frac{1}{\mathcal{Z}} \text{tr} \left(\mathcal{A} e^{-\beta \mathcal{H}} \right) \quad \text{with} \quad \mathcal{H} = - \sum_i^M H_i \quad (2.38)$$

where M is the total number of local operators in the Hamiltonian and the minus sign is for convenience as before. This average is written in the Taylor expanded formalism by using the Eq. (2.17) as following,

$$\langle \mathcal{A} \rangle = \frac{1}{\mathcal{Z}} \sum_{n=0} \frac{\beta^n}{n!} \sum_{\alpha} \sum_{\{l\}} \left\langle \alpha \left| \mathcal{A} \prod_i^n H_{l_i} \right| \alpha \right\rangle. \quad (2.39)$$

Here we use the index l to indicate a local operator term H_l . By using the definition of the weight function in Eq. (2.20) the estimator for the expectation value of the operator $\mathcal{A}$ can be written in the following form

$$\langle \mathcal{A} \rangle = \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_n} \mathcal{A}(\alpha, S_n) \mathcal{W}(\alpha, S_n) = \langle \mathcal{A}(\alpha, S_n) \rangle_{\mathcal{W}} \quad (2.40)$$

provided that function $\mathcal{A}(\alpha, S_n)$ can be found explicitly. With a configuration (α, S_n) at hand, we can regard each propagated state $|\alpha(p)\rangle$ in this configuration as the starting state $|\alpha(0)\rangle$, i.e. permute cyclically, then we have the possibility to have at most n different valid spin states over which we can make an internal average to improve the statistics of the estimator. Thus we have a weight $\mathcal{W}[\alpha(p), S_n(p)]$ for each propagated state and the estimator of $\mathcal{A}$ is written as

$$\langle \mathcal{A} \rangle = \left\langle \frac{1}{n} \sum_{p=0}^{n-1} \mathcal{A}[\alpha(p), S_n(p)] \right\rangle_{\mathcal{W}} \quad (2.41)$$

where $S_n(p)$ is the operator sequence permuted cyclically p times from $S_n = S_n(0)$. From now on we will drop the subscript $\mathcal{W}$ for brevity. Simple estimators for the SSE QMC method can be derived from this formulation. The estimators are quite simple for diagonal operators, $\mathcal{A} |\alpha\rangle = a(\alpha) |\alpha\rangle$. We prefer to show intermediate steps of the expressions, so similar equations are written repeatedly. The expectation value for the diagonal operator is written as below

$$\langle \mathcal{A} \rangle = \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_n} a(\alpha) \frac{\beta^n}{n!} \left\langle \alpha \left| \prod_i^n H_{l_i} \right| \alpha \right\rangle \quad (2.42)$$

which is in the form of Eq. (2.40) with $\mathcal{A}(\alpha, S_n) = a(\alpha)$ and the estimator for the diagonal operator $\mathcal{A}$ is given as

$$\langle \mathcal{A} \rangle = \left\langle \frac{1}{n} \sum_{p=0}^{n-1} a[\alpha(p)] \right\rangle. \quad (2.43)$$

For the general case, the form of Eq. (2.40) is researched for the estimator. We first consider the expectation value of a local operator $\mathcal{A} = H_k$,

$$\begin{aligned} \langle \mathcal{A} \rangle &= \langle H_k \rangle = \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_n} \frac{\beta^n}{n!} \left\langle \alpha \left| H_k \prod_i^n H_{l_i} \right| \alpha \right\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_{n+1}} \frac{\beta^n}{n!} \left\langle \alpha \left| \prod_i^{n+1} H_{l_i} \right| \alpha \right\rangle \delta_{l_{n+1}, k} \\ &= \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_n} \frac{\beta^n}{n!} \frac{n}{\beta} \left\langle \alpha \left| \prod_i^n H_{l_i} \right| \alpha \right\rangle \delta_{l_n, k} \end{aligned} \quad (2.44)$$

in which the second line is a sum for all possible products of $n + 1$ local operators but disregards the sequences in which the H_k is not at the leftmost place. In other words, the local operator H_k is inserted into the operator string making its length $n + 1$ but the position of the local operator H_k is fixed at the first place of the operator string S_{n+1} . In the third line, the substitution $n \leftarrow n - 1$ is performed to see the correspondence with Eq. (2.40). Thus we have $\mathcal{A}(\alpha, S_n) = \frac{n}{\beta} \delta_{l_n, k}$. The average of H_k is obtained

$$\langle H_k \rangle = \left\langle \frac{1}{n} \sum_{p=0}^{n-1} \mathcal{A}[\alpha(p), S_n(p)] \right\rangle = \frac{1}{\beta} \left\langle \sum_{p=0}^{n-1} \delta_{l_n(p), k} \right\rangle = \frac{1}{\beta} \langle \mathcal{N}(k) \rangle \quad (2.45)$$

in which $\mathcal{N}(k)$ is the number of indices k in a selected sequence and $l_i(p)$ is the index of i -th operator in the operator string that is permuted p times. With this information,

$$\langle \mathcal{H} \rangle = - \sum_k^M \langle H_k \rangle = - \frac{1}{\beta} \sum_k^M \langle \mathcal{N}(k) \rangle = - \frac{1}{\beta} \left\langle \sum_k^M \mathcal{N}(k) \right\rangle = - \langle n \rangle / \beta \quad (2.46)$$

which is exactly the same estimator Eq. (2.14). For the product of operators, the estimator is calculated similarly,

$$\begin{aligned}
\left\langle \prod_j^m H_{k_j} \right\rangle &= \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_n} \frac{\beta^n}{n!} \left\langle \alpha \left| \prod_j^m H_{k_j} \prod_i^n H_{l_i} \right| \alpha \right\rangle \\
&= \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_{n+m}} \frac{\beta^n}{n!} \left\langle \alpha \left| \prod_i^{n+m} H_{l_i} \right| \alpha \right\rangle \prod_j^m \delta_{l_{n+j}, k_j} \\
&= \frac{1}{\mathcal{Z}} \sum_{n=0} \sum_{\alpha} \sum_{S_n} \frac{\beta^n}{n!} \frac{n!}{\beta^m (n-m)!} \left\langle \alpha \left| \prod_i^n H_{l_i} \right| \alpha \right\rangle \prod_j^m \delta_{l_{n-m+j}, k_j}
\end{aligned} \tag{2.47}$$

in which in the last line the substitution $n \leftarrow n - m$ is performed to see the accordance with Eq. 2.43 as

$$\mathcal{A}(\alpha, S_n) = \frac{n!}{\beta^m (n-m)!} \prod_i^m \delta_{l_{n-m+i}, k_i} \tag{2.48}$$

and the estimator is given

$$\begin{aligned}
\left\langle \prod_j^m H_{k_j} \right\rangle &= \frac{1}{\beta^m} \left\langle \frac{(n-1)!}{(n-m)!} \sum_{p=0}^{n-1} \prod_i^m \delta_{l_{n-m+i(p)}, k_i} \right\rangle \\
&= \frac{1}{\beta^m} \left\langle \frac{(n-1)!}{(n-m)!} \mathcal{N}(k_1, k_2 \dots k_m) \right\rangle
\end{aligned} \tag{2.49}$$

where $\mathcal{N}(k_1, k_2 \dots k_m)$ is the number of operators *ordered* in the operator string S_n . We can use Eq. (2.49) to derive an expression for specific heat estimator. We already know $\langle \mathcal{H} \rangle$ from Eq. (2.46) and we can calculate $\langle \mathcal{H}^2 \rangle$ as,

$$\langle \mathcal{H}^2 \rangle = \sum_{k,l} \langle H_k H_l \rangle - \frac{1}{\beta^2} \left\langle (n-1) \sum_{k,l} \mathcal{N}(k, l) \right\rangle = \frac{1}{\beta^2} \langle (n-1)n \rangle \tag{2.50}$$

which gives the specific heat estimator,

$$C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle. \tag{2.51}$$

Static susceptibilities can be evaluated by constructing estimators from the Kubo integral

$$\chi_{AB} = \int_0^\beta d\tau \langle A(\tau) B(0) \rangle \tag{2.52}$$

where the integrand shows the ensemble average of an imaginary-time dependent product with operators $A(\tau) = e^{\tau\mathcal{H}} A(0) e^{-\tau\mathcal{H}}$. We first calculate the estimator for the integrand and then integrate it. The trace is written and then Taylor series expanded,

$$\begin{aligned}\langle A(\tau)B(0) \rangle &= \frac{1}{\mathcal{Z}} \sum_{\alpha} \left\langle \alpha \left| e^{\tau\mathcal{H}} A(0) e^{-\tau\mathcal{H}} B(0) e^{-\beta\mathcal{H}} \right| \alpha \right\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{\alpha} \left\langle \alpha \left| e^{(\tau-\beta)\mathcal{H}} A(0) e^{-\tau\mathcal{H}} B(0) \right| \alpha \right\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{\alpha} \sum_{n=0} \sum_{m=0} \frac{(\tau-\beta)^n (-\tau)^m}{n! m!} \langle \alpha | \mathcal{H}^n A \mathcal{H}^m B | \alpha \rangle\end{aligned}\quad (2.53)$$

where the second line is written by using the cyclic property of the trace and $A = A(0)$. Infinite double sums can be transformed into the infinite sums of finite series,

$$\sum_{n=0} \sum_{m=0} C_{n,m} = \sum_{n=0} \sum_{m=0}^n C_{n-m,m} \quad (2.54)$$

which can be used to make a correspondence with Eq. (2.43). By using Eq. 2.54 the integrand is written as follows,

$$\begin{aligned}\langle A(\tau)B(0) \rangle &= \frac{1}{\mathcal{Z}} \sum_{\alpha} \sum_{n=0} \sum_{m=0}^n \frac{(\tau-\beta)^{n-m} (-\tau)^m}{(n-m)! m!} \langle \alpha | \mathcal{H}^{n-m} A \mathcal{H}^m B | \alpha \rangle \\ &= \frac{1}{\mathcal{Z}} \sum_{\alpha} \sum_{n=0} \sum_{m=0}^n \sum_{S_n} \frac{\tau^m (\beta-\tau)^{n-m}}{(n-m)! m!} \left\langle \alpha \left| \prod_{i=m+1}^n H_{l_i} A \prod_{j=1}^m H_{l_j} B \right| \alpha \right\rangle\end{aligned}\quad (2.55)$$

which will be handled for both diagonal or non-diagonal cases of A and B . Note that, we should remember the sign convention for $\mathcal{H} = -\sum_i^M H_i$ which produces a factor $(-1)^n$ from going the first line to the second line, and it is absorbed into the variables. For the diagonal cases of A and B the state is propagated and back-propagated as,

$$A \prod_i^m H_{l_i} B | \alpha \rangle = a[\alpha(m)] b[\alpha(0)] | \alpha(m) \rangle = a[\alpha(m)] b[\alpha(0)] \prod_i^m H_{l_i} | \alpha \rangle \quad (2.56)$$

and replaced into Eq. (2.55),

$$\langle A(\tau)B(0) \rangle = \frac{1}{\mathcal{Z}} \sum_{\alpha} \sum_{n=0} \sum_{m=0}^n \sum_{S_n} \frac{\tau^m (\beta-\tau)^{n-m}}{(n-m)! m!} a[\alpha(m)] b[\alpha(0)] \left\langle \alpha \left| \prod_i^n H_{l_i} \right| \alpha \right\rangle \quad (2.57)$$

from which we extract

$$\mathcal{A}(\alpha, S_n) = \sum_{m=0}^n \frac{\tau^m (\beta - \tau)^{n-m} n!}{(n-m)! m! \beta^n} a[\alpha(m)] b[\alpha(0)] \quad (2.58)$$

that leads to the estimator for the integrand when A and B are diagonal,

$$\langle A(\tau) B(0) \rangle = \left\langle \sum_{p=0}^{n-1} \sum_{m=0}^n \frac{\tau^m (\beta - \tau)^{n-m} (n-1)!}{(n-m)! m! \beta^n} a[\alpha(p+m)] b[\alpha(p)] \right\rangle \quad (2.59)$$

in which the eigenvalues a and b are always from the states that are separated by m positions due to the periodicity of the imaginary time direction.

Before performing the integral of Eq. (2.59), we investigate another case by replacing $A = H_{k_1}$ and $B = H_{k_2}$ into Eq. (2.55):

$$\begin{aligned} \langle H_{k_1}(\tau) H_{k_2}(0) \rangle &= \frac{1}{\mathcal{Z}} \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{m=0}^n \sum_{S_{n+2}} \frac{\tau^m (\beta - \tau)^{n-m}}{(n-m)! m!} \left\langle \alpha \left| \prod_i^{n+2} H_{l_i} \right| \alpha \right\rangle \delta_{l_1, k_1} \delta_{l_{m+2}, k_2} \\ &= \frac{1}{\mathcal{Z}} \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{m=0}^{n-2} \sum_{S_n} \frac{\tau^m (\beta - \tau)^{n-m-2}}{(n-m-2)! m!} \left\langle \alpha \left| \prod_i^n H_{l_i} \right| \alpha \right\rangle \delta_{l_1, k_1} \delta_{l_{m+2}, k_2} \end{aligned} \quad (2.60)$$

in which the second line is produced from the first line by the substitution $n \leftarrow n - 2$ to see the correspondence with Eq. (2.43), i.e.,

$$\mathcal{A}(\alpha, S_n) = \frac{\tau^m (\beta - \tau)^{n-m-2} n!}{(n-m-2)! m! \beta^n} \delta_{l_1, k_1} \delta_{l_{m+2}, k_2} \quad (2.61)$$

gives the estimator for the products of the imaginary-time dependent operators,

$$\begin{aligned} \langle H_{k_1}(\tau) H_{k_2}(0) \rangle &= \left\langle \sum_{m=0}^{n-2} \frac{\tau^m (\beta - \tau)^{n-m-2} (n-1)!}{(n-m-2)! m! \beta^n} \sum_{p=0}^{n-1} \delta_{l_1(p), k_1} \delta_{l_{m+2}(p), k_2} \right\rangle \\ &= \left\langle \sum_{m=0}^{n-2} \frac{\tau^m (\beta - \tau)^{n-m-2} (n-1)!}{(n-m-2)! m! \beta^n} \mathcal{N}(k_1, k_2; m) \right\rangle \end{aligned} \quad (2.62)$$

where $\mathcal{N}(k_1, k_2; m)$ is the number that how many times the indices k_1 and k_2 are ordered and separated by m positions in the operator string S_n .

Now it is time to perform the Kuba integral for which the only required integration formula is,

$$\int_0^\beta d\tau \tau^m (\beta - \tau)^{n-m} = \frac{\beta^{n+1} m! (n-m)!}{(n+1)!} \quad (2.63)$$

which can be proven by using integration by parts and mathematical induction. Then we integrate the Eq. (2.59) and simplify it as follows,

$$\begin{aligned} \int_0^\beta d\tau \langle A(\tau) B(0) \rangle &= \left\langle \sum_{p=0}^{n-1} \sum_{m=0}^n \frac{\beta}{n(n+1)} a[\alpha(p+m)] b[\alpha(m)] \right\rangle \\ &= \left\langle \frac{\beta}{n(n+1)} \left[\sum_{p=0}^{n-1} a[\alpha(p)] b[\alpha(p)] + \sum_{p=0}^{n-1} b[\alpha(p)] \sum_{m=1}^n a[\alpha(p+m)] \right] \right\rangle \\ &= \left\langle \frac{\beta}{n(n+1)} \left[\sum_{p=0}^{n-1} a[\alpha(p)] b[\alpha(p)] + \left(\sum_{p=0}^{n-1} b[\alpha(p)] \right) \left(\sum_{p=0}^{n-1} a[\alpha(p)] \right) \right] \right\rangle \end{aligned} \quad (2.64)$$

where in the second line the term for $m = 0$ is separated and in the third line the sum over m is taken out of the sum over p because the sum $\sum_m^n a[\alpha(p+m)]$ is the same for all p . The third line is a very simple estimator to implement in an SSE algorithm. For the conserved quantity S^z , Eq. (2.64) reduces to uniform susceptibility with $a[\alpha(p)] = b[\alpha(p)] = S^z$,

$$\chi_u = \beta \langle (S^z)^2 \rangle \quad (2.65)$$

and for the quantity staggered magnetization with $a[\alpha(p)] = b[\alpha(p)] = m_s[\alpha(p)]$

$$\chi_s = \left\langle \frac{\beta}{n(n+1)} \left[\sum_{p=0}^{n-1} m_s^2[\alpha(p)] + \left(\sum_{p=0}^{n-1} m_s[\alpha(p)] \right)^2 \right] \right\rangle. \quad (2.66)$$

The staggered structure factor is related to the staggered magnetization and is calculated as,

$$\mathcal{S}(\pi) = N \left\langle \sum_{p=0}^{n-1} m_s^2[\alpha(p)] \right\rangle. \quad (2.67)$$

For the more general case, Eq. (2.62), the Kubo integral is performed in the same way with the substitution $n \leftarrow n - 2$ in the Eq. (2.63). The integration formula is applied to the first line of Eq. (2.62) because the explicit m dependence cancels out and this has

the advantageous to further simplify the estimator:

$$\begin{aligned} \int_0^\beta d\tau \langle H_{k_1}(\tau) H_{k_2}(0) \rangle &= \frac{1}{\beta} \left\langle \sum_{p=0}^{n-1} \delta_{l_1(p), k_1} \sum_{m=0}^{n-2} \delta_{l_{m+2}(p), k_2} \right\rangle \\ &= \frac{1}{\beta} \left\langle - \sum_{p=0}^{n-1} \delta_{l_1(p), k_1} \delta_{l_1(p), k_2} + \sum_{p=0}^{n-1} \delta_{l_1(p), k_1} \sum_{m=0}^{n-1} \delta_{l_{m+2}(p), k_2} \right\rangle \end{aligned} \quad (2.68)$$

where the second line is written by adding and removing a term $\delta_{l_{n+1}(p), k_2} = \delta_{l_1(p), k_2}$ to the summation over m in the first line. The sum over m in the second line is the same for all p and goes out of the summation over p . Thus we can write the estimator of the Kubo integral of two local Hamiltonian operators (any two instances of Eq. (2.30a) and Eq. (2.30b)) as in the following simple form,

$$\int_0^\beta d\tau \langle H_{k_1}(\tau) H_{k_2}(0) \rangle = [\langle \mathcal{N}(k_1) \mathcal{N}(k_2) \rangle - \langle \mathcal{N}(k_1) \delta_{k_1, k_2} \rangle] / \beta. \quad (2.69)$$

As an important application of Eq. (2.69), an estimator that can measure the spin stiffness can be derived. Spin stiffness is related to the spin current operator J_s (Avella & Mancini, 2013),

$$J_s = -i \sum_j (S_j^+ S_{j+1}^- - S_j^- S_{j+1}^+) \quad (2.70)$$

such that we need to compute the following average,

$$\int_0^\beta d\tau \langle J_s(\tau) J_s(0) \rangle. \quad (2.71)$$

The spin current operator is not exactly in the form of the off-diagonal local operator of Eq. (2.30b). First, we realize that only one of the terms in the off-diagonal local operator ($S_j^+ S_{j+1}^-$ or $S_j^- S_{j+1}^+$) gives contribution to the weight of the configuration and the effect of each contribution is to transport a spin in a negative or positive direction. So total number of off-diagonal operators in an operator string can be calculated by counting the number of operators transporting the spin. This property enables to calculate the differences between the number of operators transporting spin in positive and negative directions. Thus we can write,

$$\int_0^\beta d\tau \langle J_s(\tau) J_s(0) \rangle = \left(\langle [N(+) - N(-)]^2 \rangle - \langle N(+) - N(-) \rangle \right) / \beta \quad (2.72)$$

where $\mathcal{N}(+)$ ($\mathcal{N}(-)$) is the number of operators transporting spin in the positive (negative) direction. Spin stiffness ρ_s is related to a twist angle ϕ imposed to a boundary of spins. We now write the definition and the estimator for spin stiffness,

$$\rho_s = \frac{1}{N} \left. \frac{\partial^2 F(\phi)}{\partial \phi^2} \right|_{\phi=0} = \frac{1}{\beta N} \langle [\mathcal{N}(+) - \mathcal{N}(-)]^2 \rangle \quad (2.73)$$

where $F(\phi)$ is the free energy of the twisted system and the last term of Eq. (2.72) cancels with a term coming from the second the derivative of the partition function of the twisted system (the first derivative vanish due to the symmetry). The form of the estimator for the spin stiffness is the same for both SSE QMC and PIMC methods (Avella & Mancini, 2013). The total number of times a spin is transported along a spatial dimension is a measure of how many times the spin wraps around the boundary of that dimension. So the spin stiffness is related to a topological quantity called *winding number* to which the SSE QMC method can directly access and for that reason the spin stiffness is a good quantity to extract critical exponents of a quantum spin system.

CHAPTER THREE

TWO-LEG LADDERS WITH BIMODAL DISORDER

The link between the low-dimensional systems and the superconductivity makes quantum spin systems an attractive research area even in one dimension with antiferromagnetic interactions (Vasiliev et al., 2018). A gapped spectrum in an integer spin chain with antiferromagnetic interactions has been conjectured by Haldane and supported by many studies (Affleck & Lieb, 1986; Buyers et al., 1986; Nightingale & Blöte, 1986). Later the chains have been coupled to each other and the so-called ladder systems have been constructed. The spectrum of the ladder systems with an even number of legs (chains) and half-integer spins has been predicted to be gapped by the observation of exponentially decaying spin-spin correlation and spin susceptibility (Dagotto & Rice, 1996). A finite gap is present for any antiferromagnetic exchange interaction in a ladder system with an even number of legs. The value of the gap can be extracted by using the low-temperature form of the uniform susceptibility (Frischmuth et al., 1996; Sandvik, 2010a; White, 1996),

$$\chi(T) \sim T^{-1/2} e^{-\Delta/T} \quad (3.1)$$

where T is the temperature and the Δ is the spin gap. For a two-leg ladder with isotropic antiferromagnetic exchange interactions the gap can easily be calculated by QMC method in a few seconds approximately as $0.5J$ (Barnes et al., 1993). In this chapter, the Eq. (3.1) is linearized and the value of the gap is extracted by making a least square fit to it.

The value of the gap can be changed by extending the simple ladder models to more complicated ones. Bonds disorder is one of the modifications that can be applied on the pure ladder model (Mélin et al., 2002). Other than this, the interactions can include frustration (Maiti et al., 2018; Metavitsiadis & Eggert, 2017), and an external magnetic field can be applied (Chitra & Giamarchi, 1997). Importantly, a light doping with non-magnetic impurities can considerably reduce the value of gap (Iino & Imada, 1996; Korenblit, 1997; Lavarélo et al., 2013; Mikeska et al., 1997; Motome et al., 1996; Nagaosa et al., 1996). Motome et al. (1996) put forward a quantum phase transition

in a ladder system and Nagaosa et al. (1996) discover a Berry phase term by treating the ladder system as a spin liquid. The magnetic field can affect the ladders remarkably such that the gap can be destroyed at a critical value or the ladder can be made fully saturated for another critical field (Chitra & Giamarchi, 1997; Giamarchi & Tsvelik, 1999; Rüegg, Kiefer, et al., 2008; Wessel, Olshanii, et al., 2001).

There are a different number of ladder models such as ladders with dimerization (Cabra & Grynberg, 2000; J. Chen et al., 2012; Q.-H. Chen et al., 2014; Jahangiri et al., 2017; Japaridze & Mahdavifar, 2009; Kariyado & Hatsugai, 2015; Shahri Naseri & Mahdavifar, 2017), zigzag ladders (Bunder & Lin, 2009; S. Chen et al., 2001; Danilovich et al., 2017; Hoyos & Miranda, 2004; Maiti et al., 2018), mixed ladders (Aristov & Kiselev, 2004; Batchelor et al., 2001; Batchelor et al., 2004; Kolezhuk & Mikeska, 1998; Zad & Ananikian, 2018), etc. Several different methods are available to investigate the ladder models. A few examples are ED, DMRG, spin-wave theory, and bosonization (Aristov & Kiselev, 2004; Maiti et al., 2018). Disordered models are in demand recently. The sensitivity of weakly disordered anisotropic ladders has been investigated (Orignac & Giamarchi, 1998). On the opposite side, the strong disorder has been studied with the strong disorder renormalization group and DMRG methods (Iglói & Monthus, 2005; Mélin et al., 2002; T. Vojta, 2013).

As explained in detail, the QMC simulation will be a powerful method to compute important properties of the ladder systems in the presence of disorder. An antiferromagnetic spin-1/2 Heisenberg ladder in the presence of bond disorder has been studied by the SSE QMC technique and the neighboring bond energies have been detected to depend on the location of the disorder (Trinh & Haas, 2013).

Bond disordered ladders have recently been investigated (Trinh & Haas, 2013) by the very efficient SSE QMC technique and in a similar bond disordered model, dynamic properties of quantum spin ladders have been studied (Hörmann et al., 2018). In Ref. Trinh and Haas (2013), quantum phases of a bond disordered antiferromagnetic spin-1/2 Heisenberg ladder have been studied in the presence of a magnetic field and they have found that the position of disorder has considerable changes on the neighbouring

bond energies. In a more recent study, Hörmann et al. (2018) introduced a disorder to a spin-1/2 antiferromagnetic ladder model only along the rung and only along the leg directions. They have observed the disorder affects the collective excitations by calculating the dynamic structure factor. Consequently, the static properties of this ladder model are lacking in the literature. In this chapter we search the properties of a two-leg spin-1/2 ladder system with a bimodal disorder along only the rung direction.

As a result, we use the SSE QMC method with operator loops to calculate the thermodynamic properties for different disorder strengths. The calculations showed a decreasing spin gap with increasing disorder parameter and a crossing point has been detected at which the disorder does not affect the results for both specific heat and uniform susceptibility.

In the next section, we give the details of the model. The results are given from the clean to the fully disorder limits for antiferromagnetic interactions at finite temperatures. Spin gaps have been evaluated which requires computations at low temperatures. We compare the results with the clean case of the system. In the last section, we conclude the results with important findings.

3.1 Model and the Simulation Details

For the Hamiltonian of the quantum spin ladder model, Eq. (2.29) can be used with suitably selected exchange interactions and bonds. In a two-leg ladder system with N sites there are $N_b = 3N/2$ bonds. For the present model all the bonds have an antiferromagnetic exchange interaction, i.e., all $J_b > 0$. We label the first N bonds to be along the legs with $J_b = J$ and label the remaining $N/2$ bonds along the rung with $J_b = J_+$ or $J_b = J_-$. The interaction in the randomly selected half of the bonds along the rung ($N/4$ bonds) is assigned to J_+ (or J_-) and the remaining half of the bonds are assigned to J_- (or J_+). The coupling constants along the rung satisfy the condition $(J_+ + J_-)/2J = 1$. A specific and small realization of the system is shown in Figure 3.1 as a reference. In other words, the bonds along the rungs are selected from a more

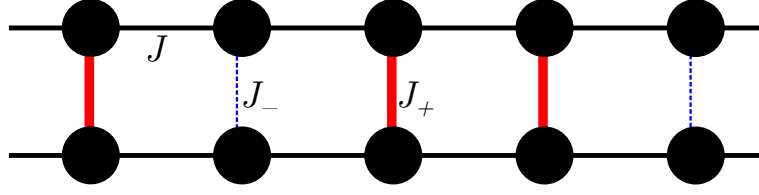


Figure 3.1 An example two-leg ladder lattice with a bimodal disorder configuration. Solid (red) and dashed (blue) lines are the bond interaction energies J_+ and J_- respectively that satisfy the condition $(J_+ + J_-)/2 = 1$. All the couplings along the legs are the same (J)

general bimodal distribution

$$\mathcal{P}(J_b) = p\delta(J_b - J_+) + (1 - p)\delta(J_b - J_-) \quad (3.2)$$

with probability $p = 1/2$. For this problem we use $L_x = 256$ sites for a single leg throughout the simulations so the total number of sites is $N = L_x \times 2$. To measure the strength of the disorder we define a parameter ρ as $J_{\pm} = 1 \pm \rho$ where $J_+ > 1$ and $J_- < 1$ for all values of $0 \leq \rho \leq 1$. It is obvious $\rho = 0$ is the clean case of the system.

We measure the quantities of interest for ten different disorder strengths and for the clean case such that $\rho = 0.0, 0.1, 0.2, \dots, 0.9, 1.0$. The temperature is changed from the vicinity of zero to $T/J = 2$ by a fixed step. At some temperatures the results seemed to be independent of the disorder so a fine sweeping around those temperatures was performed. A thousand of random realizations were generated and the same configurations were used for all temperature values. Each disorder configuration is used as a bin each consisting 5×10^5 MCS after discarding 5×10^4 MCS for the data analysis. For the simulations around special temperature points, 10^6 MCS were performed. The sufficiency of the number of disorder configurations was ensured by performing running averages of uniform susceptibility and the specific heat in the vicinity of crossing points and broad maximums. To get a good statistics the standard errors for nonlinear functions have been propagated with the Bootstrap resampling technique.

3.2 Results and Discussion

The results for all disorder strengths are around the clean case. While the disorder did not create a completely different physical behavior we realized a special temperature point for specific heat and another special temperature point for the uniform susceptibility. The values of uniform susceptibility and the specific heat are independent of the disorder parameter at their special temperature points and they cross. A fine sweeping in the vicinity of these temperature points was performed and the existence of crossing points was determined up to some precision.

A Curie behavior is present for the uniform susceptibility (χ_u) results at high temperatures as shown in the Figure 3.2. The broad maximums of the uniform susceptibility shift left with increasing disorder strength. At low temperatures, there is an exponential decrease that is a sign of the gap for all disorder strengths.

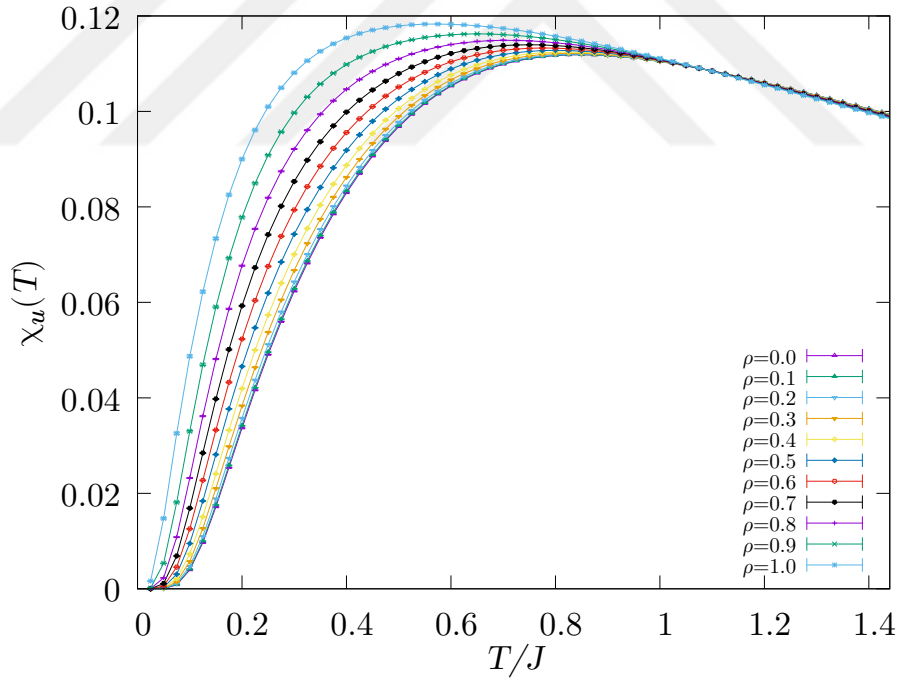


Figure 3.2 Uniform susceptibility for all disorder strengths together with the clean case for reference. For high temperatures a Curie behavior is present and for low temperatures, there is an exponential decay indicating a spin gap for all disorder strengths. The lines are guide to the eye

For uniform susceptibility, the crossing point is located at the right side of the broad maximums. The crossing point is calculated using the pairs of disorder strengths

separated by three tenths, i.e., by pairs $(\rho, \rho + 0.3)$: $(0, 0.3)$, $(0.1, 0.4)$, $(0.2, 0.5)$, $(0.3, 0.6)$, $(0.4, 0.7)$, $(0.5, 0.8)$, $(0.6, 0.9)$ and $(0.7, 1.0)$. In this way, we calculate the crossing point for uniform susceptibility as 1.083(3). The corresponding value of this crossing point for the uniform susceptibility is $\chi_u^* = 0.1088(1)$. Parallel outcomes have been recorded for magnetic spin susceptibilities in the spin-1/2 stacked 2-leg ladder systems (Johnston et al., 2000).

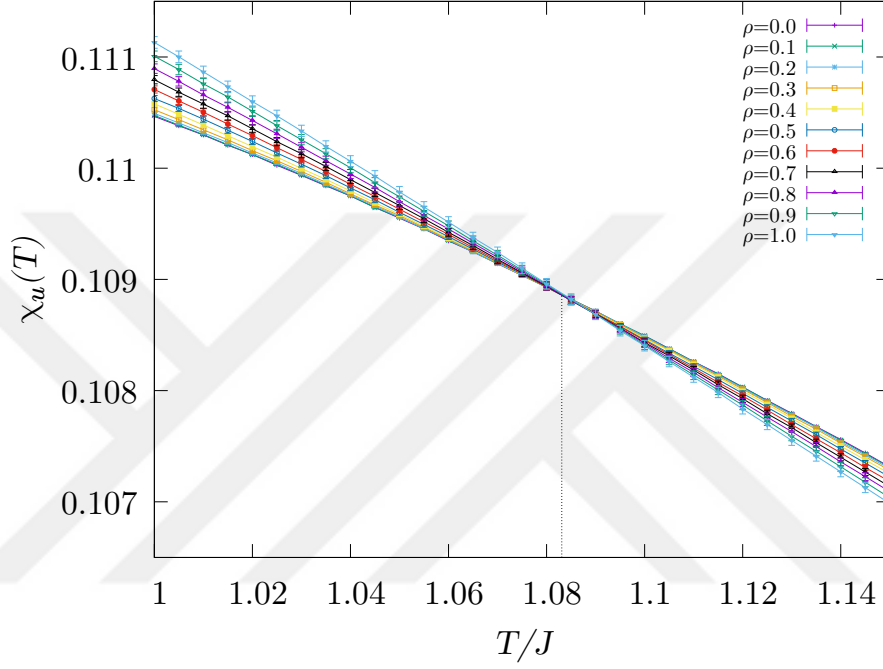


Figure 3.3 Fine sweeping around the crossing point of uniform susceptibility. The location of the crossing point is indicated by the vertical dashed line: 1.083. The lines are guide to the eye

Contrary to uniform susceptibility, the maximums of heat capacity decrease with increasing disorder strength parameters as shown in the Figure 3.4. The crossing point is more apparent for that quantity as shown in the Figure 3.5 which displays the fine sweeping for specific heat. By using the same pairs of disorder strengths the crossing point for the specific heat is calculated as 0.9453(3). The specific heat value corresponding to the crossing point is found as $C^* = 0.2912(7)$. The crossing points for specific heat and the uniform susceptibility are close to each other. To be sure that the crossing points are distinct we employed simulations for the larger system size $L_x = 512$ and found the same results so the crossing points are size-independent. They are not critical points so we called them special (or crossing) points. We can say that this system exhibit two different crossing points one for specific heat and one

for uniform susceptibility. Similar points have been reported in the literature either experimentally (Chandra et al., 1999; Vollhardt, 1997) or numerically (Georges & Krauth, 1993) and the specific heat was found to be independent of quantities such as pressure, magnetic field, and local Hubbard interaction. A possible reason for this behavior was investigated theoretically for both lattice and continuum models (Vollhardt, 1997) and the half-filled Hubbard model examined in all dimensions (Chandra et al., 1999). An interesting result was found by Chandra et al. (1999) that the corresponding specific heat values were calculated to have almost the same nearly universal value, $\approx 0.34/k_B$, for different crossing points of different geometries. We report here a slightly smaller value, $\approx 0.29/k_B$, for the present rung disordered Heisenberg ladder model. Vollhardt (1997) noted that at the crossing point the derivative of the specific heat with respect to the disorder strength at the crossing point changes sign to conserve the total entropy change. Mathematically the crossing point of the specific heat is an inflection point. The SSE QMC method extracts the crossing points within a good precision.

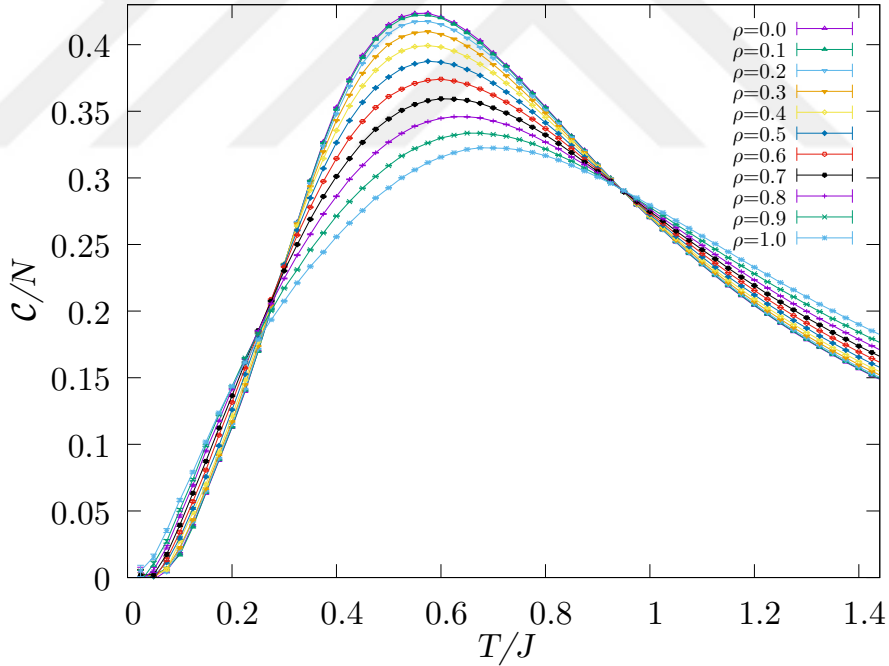


Figure 3.4 Specific heat curves for all disorder strengths. The crossing point is visible at the right side of the peaks. The lines are guide to the eye

The structure factor exhibits a peak at a temperature slightly below the spin gap (Greven et al., 1996). For the present model, the structure factor exhibits decreasing peaks with increasing disorder strengths as shown in Figure 3.6. This is a sign of

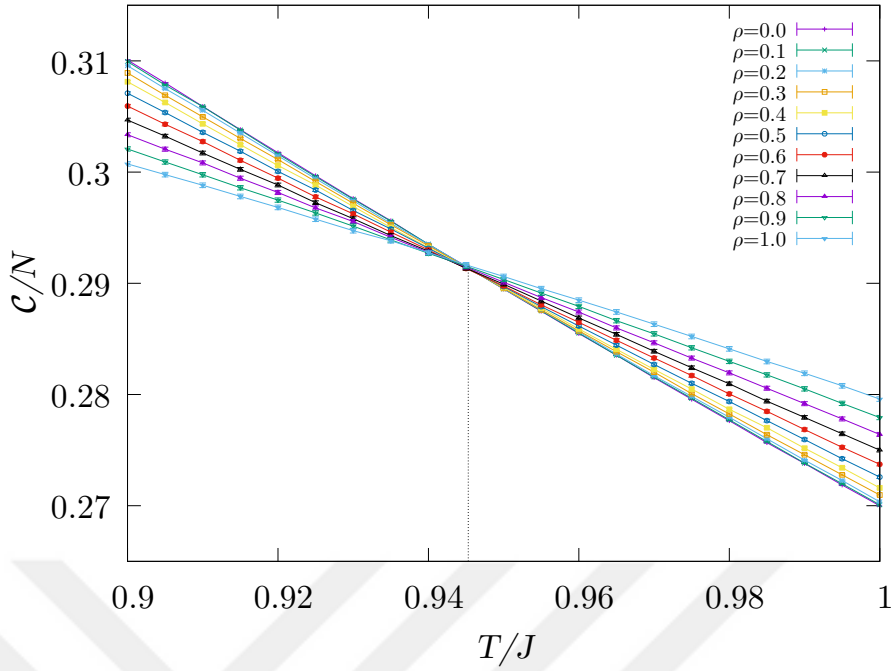


Figure 3.5 Fine sweeping of the specific heat. The existence of the crossing point is more clear. The location of the crossing point is indicated by the vertical dashed line: 0.9453. The lines are guide to the eye

decreasing spin gap with increasing disorder strength. We confirm the existence of those gaps and calculate their values by using the Eq. (3.1) at low enough temperatures. On the high-temperature regime, the results are nearly independent of the disorder and no crossing point detected on the whole investigated temperature interval.

The ground state of the clean case of the system is known to be close to a rung-dimer state (Miyazaki et al., 1997). The finite values of the staggered susceptibility down to zero temperature indicate the persistence of the ground state of the clean case for all parameters as shown in Figure 3.7. The high-temperature behavior of the staggered susceptibility is the same as previous quantities, nearly independent of the disorder parameter and no crossing point is not encountered also.

The spin gap values for all parameters are calculated by linearizing the Eq. (3.1). The low-temperature exponentially decaying behaviors of the uniform susceptibility for all disorder strengths are shown in Figure 3.8. While going to the fully disordered case the decaying pattern of uniform susceptibility change and the averages have bigger errors.

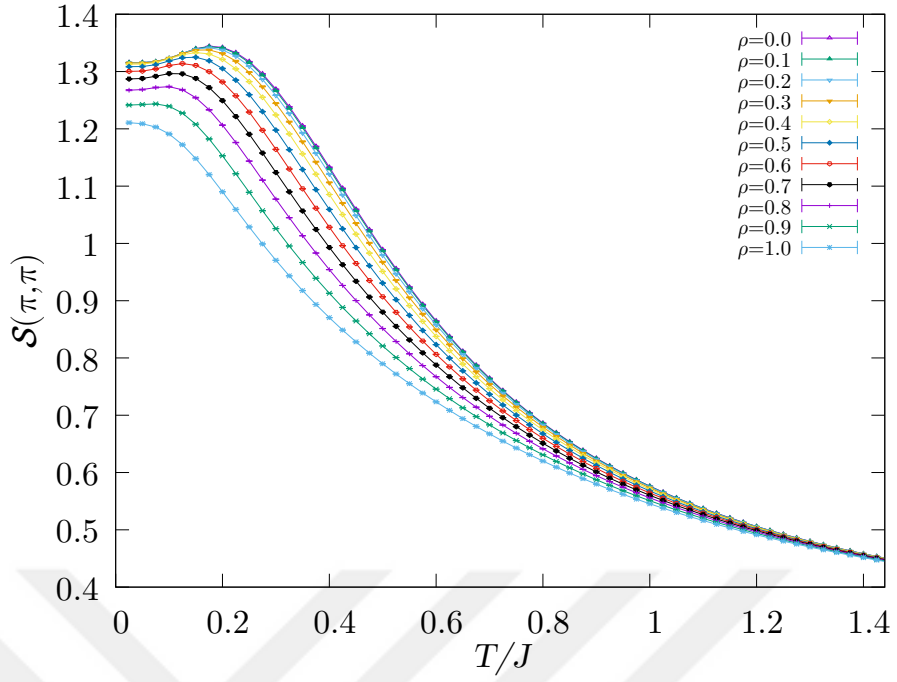


Figure 3.6 Structure factors for all disorder strengths. The peaks are evidence for the spin gaps. The lines are guide to the eye

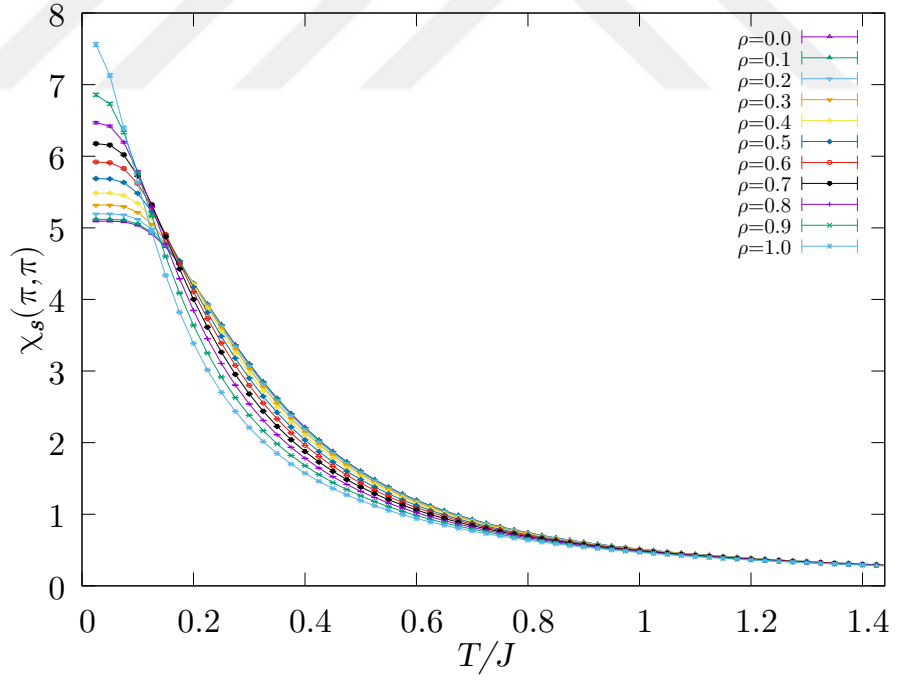


Figure 3.7 Staggered susceptibility for all disorder parameters together with the clean case of the system. The finite values of the staggered susceptibility down to zero temperature indicate that the ground state of the clean system is not affected by the disorder. The lines are guide to the eye

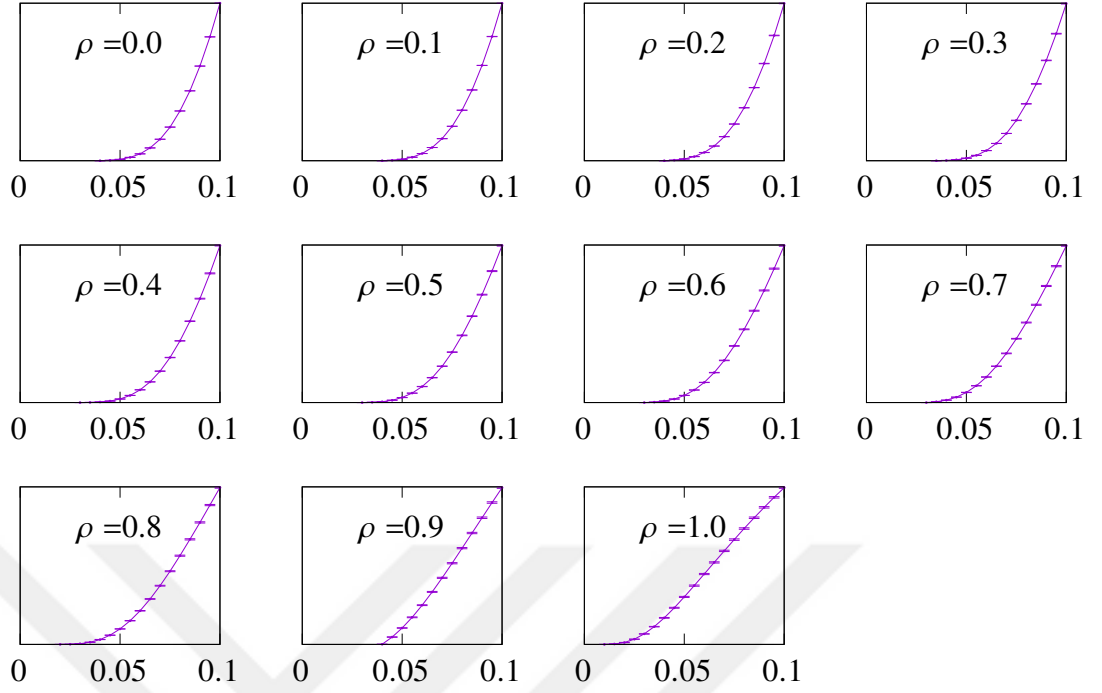


Figure 3.8 The low-temperature (x -axis) exponentially decaying behaviors of the uniform susceptibility (y -axis)

The spin gap value for the clean case ($\rho = 0$) is calculated as 0.505513(84). The gap values for other disordered cases are all below the value of the clean case in a decreasing fashion as shown in Figure 3.9. For the fully disordered case, the gap value is around $\Delta/J \approx 0.16$ which is well above the weak coupling limit (Greven et al., 1996).

The results for all quantities do not noticeably deviate from the clean case for $\rho = 0.1$. As we indicated that the spin gaps decrease with increasing disorder strength. The variation of the spin gap with disorder parameter is shown in Figure 3.10. In the middle part of the graph, it is seen that the decrease in the gap is almost linear. The decline at the tails is slow and rapid near to the clean and fully disordered cases, respectively.

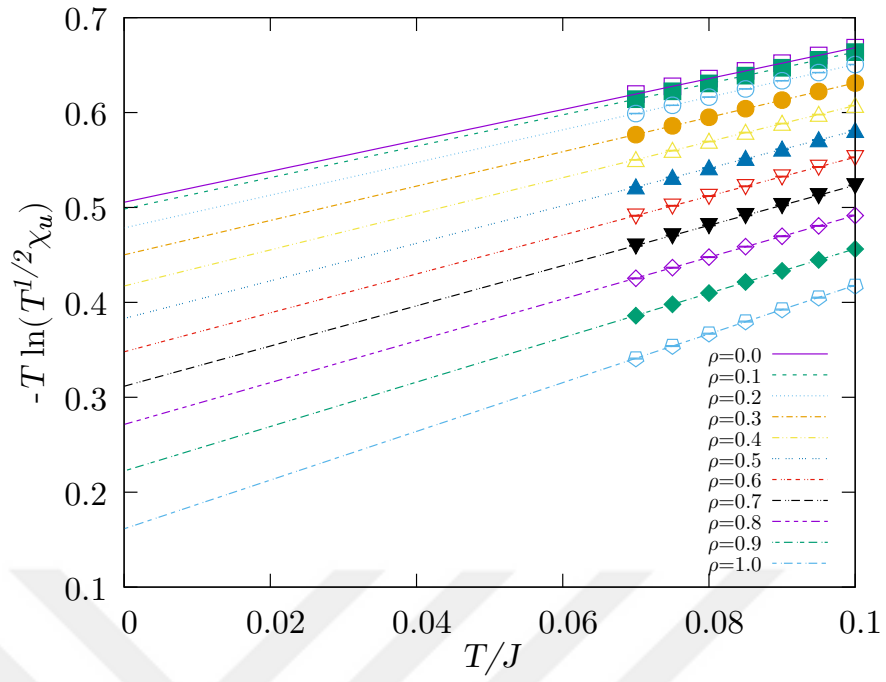


Figure 3.9 Spin gap fit lines for all disorder parameters. The gaps decrease with increasing disorder parameter. The slopes of the lines increase from top to down. The data point at $T/J = 0.1$ for $\rho = 1.0$ was excluded from the fitting

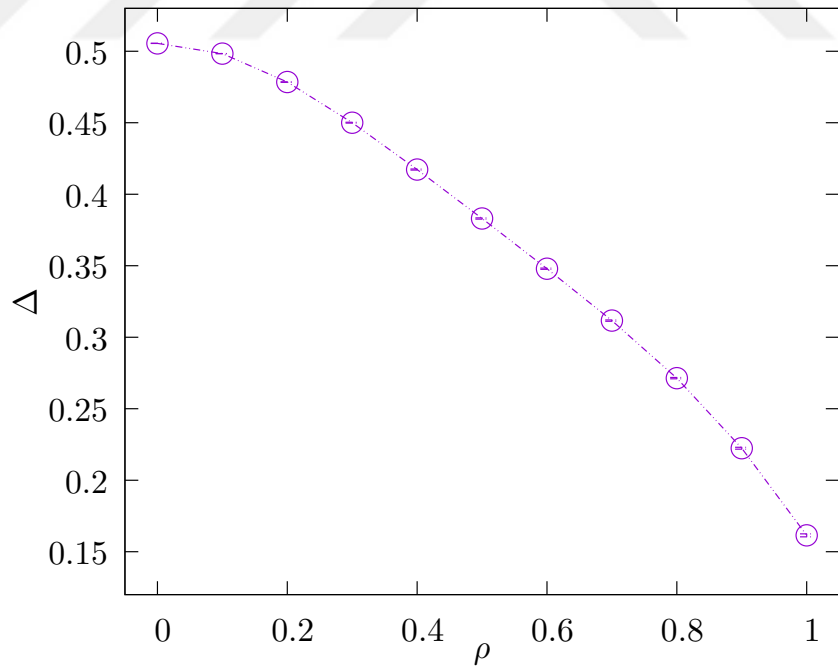


Figure 3.10 Spin gap values changing with disorder parameter. The lines are guide to the eye

CHAPTER FOUR

3D QUANTUM HEISENBERG MODEL WITH BIMODAL DISORDER

Random interactions or the disorder are important in statistical physics as well as in condensed matter physics to understand the universality concept and the criticality of magnetic materials (Chernyshev et al., 2001; Höglund & Sandvik, 2003, 2007; Ibrahim & Vojta, 2017; Laflorencie et al., 2006; Lin et al., 2006; Liu et al., 2018; Sachdev & Vojta, 2003; Sandvik, 1994, 2002b, 2006; Sandvik & Vekić, 1995; T. Vojta & Lee, 2006; T. Vojta & Schmalian, 2005; Wessel, Normand, et al., 2001; Young, 1997). The effects of disorder on the critical behavior of the second-order phase transitions have been a challenge so far. The disorder can be incorporated into the magnetic system in different ways (T. Vojta, 2019) such as introducing random magnetic interactions or fields. Real materials are not perfect and include defects in some way. Accordingly, the physical properties of materials at either zero or finite temperatures might strongly depend on the type or the strength of the disorder. The disordered systems can exhibit unconventional and different behavior from their clean counterparts (Ibrahim & Vojta, 2017; Sandvik, 2006; T. Vojta & Lee, 2006; T. Vojta & Schmalian, 2005). To give an example, T. Vojta and Schmalian (2005) showed that all critical exponents and the dynamical correlations belong to a different novel universality in the presence of a quenched disorder.

The importance of the Heisenberg model has been mentioned in the preceding chapters. One of its main roles is to build a bridge between numerical simulations and experiments. In this way, the Heisenberg model helps us to understand the physical properties of magnetic materials by enabling us to make comparisons with the experiment. Various studies include spin models with random bonds (Fabritius et al., 2010; Fisher, 1994; Frischmuth & Sigrist, 1997; Hamacher et al., 2002; Sandvik, 1994; Sandvik & Vekić, 1995; Shimokawa et al., 2015; Yasuda et al., 2002), site dilution (Behre & Miyashita, 1992; Chernyshev et al., 2001, 2002; Kato et al., 2000; Sandvik, 2001; Vajk & Greven, 2002; Wan et al., 1991; Wessel, Normand, et al., 2001; Yasuda et al., 2001; Yu et al., 2010), impurity effects (Eggert & Affleck, 1992), frustration (Albuquerque et al., 2011; Alet et al., 2016; Bishop et al., 2012; Bishop et al., 2015; Furukawa et al., 2012; Gong et al., 2015; Stapmanns et al., 2018), $J - Q$ terms (Iaizzi et al., 2017, 2018;

Liu et al., 2018; Sandvik, 2010b; Zhao et al., 2019), dimerization (Albuquerque et al., 2008; Fritz et al., 2011; Jiang, 2012; Ran et al., 2019; Wenzel et al., 2008; Wenzel & Janke, 2009; Yao et al., 2010), etc. Among these Albuquerque et al. (2008) investigated the magnetic properties of a 2D Heisenberg antiferromagnet using a QMC simulation method, and estimated the critical exponent of the correlation length as the same of the $O(3)$ classical Heisenberg universality, $\nu \approx 0.71$ (Campostrini et al., 2002; Peczak et al., 1991). Recently Wenzel and Janke (2009) have reconfirmed the value of ν by analyzing ladder and plaquette models on two dimensions with the SSE QMC method. As can be understood, there are high precision data on the universality properties of 1D and 2D systems that are either disordered or pure. Yet the universality properties of 3D quantum models with the disorder are still lacking. The reason can be linked to the vast number of sites even in small sizes in three dimensions and to the number of random realizations required. Both entail intensive computational resources on their own.

The experimental observation of TiCuCl_3 inspired many studies (Merchant et al., 2014; Rüegg et al., 2003; Rüegg, Normand, et al., 2008). Recent studies on 3D quantum antiferromagnetic systems with or without the disorder have researched the scaling relations of the staggered magnetization and Néel temperature (T_N) (Jin & Sandvik, 2012; Kao & Jiang, 2013; Kulik & Sushkov, 2011; Oitmaa et al., 2012; Tan & Jiang, 2015; Tan & Jiang, 2017, 2020; Tan et al., 2018). Jin and Sandvik (2012) related the T_N with the staggered magnetization in the ground state and measured an almost perfect universality. On a 3D random quantum antiferromagnet, Tan and Jiang (2015) examined the scaling of those quantities related to each other and reported the parallel results with the scaling relations of the clean system. The scaling relations have also been confirmed for the system with configuration disorder (Tan & Jiang, 2017). As a result, the critical behavior of the 3D quantum antiferromagnetic system is universal whether it is pure or disordered. T_N and staggered magnetization show a data collapsing behavior at the criticality, which is an important property for experimentalists. Thus the scaling relations of those quantities attempt much attention. Some questions still wait for clarification in the presence of quenched disorder. Does the disorder affect the T_N or change the universality class of the system. Or to what extent does the system conserve its critical behavior against the disorder strength? In this chapter, we use the SSE QMC method to

investigate the universality properties of Heisenberg hamiltonian defined on a 3D cubic lattice with nearest-neighbor interactions that are distributed randomly to be either J_1 or J_2 satisfying the condition $(J_1 + J_2)/2J = 1$. We try to answer the questions above. We will see that the results indicate the same universality class with the classical 3D Heisenberg model.

4.1 Model and the Simulation Details

As in the case of the quantum spin ladder, we use Eq. (2.29) to describe the present 3D quantum antiferromagnet. On a simple cubic lattice of linear size L with NN interactions and periodic boundary conditions, there are $N = L^3$ sites and $N_b = 3N$ bonds. All the bonds are the nearest neighbor interacting sites, and the interaction strengths of the bonds are selected from the bimodal distribution defined in Eq. (3.2). While the distribution is the same as with the ladder model we use a slightly different convention here. Half of the bonds interact with energy J_1 and the rest half interact with energy J_2 the constraint $(J_1 + J_2)/2J = 1$ is imposed. We define the disorder strength as $r = J_2/J_1$ and $r = 1$ is the clean (pure) case of the 3D spin-1/2 antiferromagnetic Heisenberg model. The critical temperature of the clean system predicted by QMC simulations is between $k_B T_N/J = 0.946(1)$ (Sandvik, 1998) and 0.947 (Troyer et al., 2003).

The linear size L of the system has the values $L = 4, 6, 8, 10, 12, 14, 16, 18, 20, 24, 28, 32, 36$, and 48. The simulations were performed for three different disorder strengths namely $r = 0.9/1.1, 0.75/1.25$, and $0.5/1.5$. It should be stressed that the strength of disorder is more strong for the values of r far from 1. For each parameter set (L, r) , 300 random independent realizations were generated and used in the temperature range considered. For each disorder realization, a total of 6×10^5 MCSs were performed of which the first 10^5 is discarded for the saturation process. Each random realization was used as a bin for the desired statistical analysis and the sufficiency of the total number of realization was assured by making a running average of the specific heat for the largest system size and strongest disordered case near the critical temperature as shown in the Figure 4.1. It is apparent from Figure 4.1 that 300 random disorder configurations are enough for good statistics. Similar analyses were performed for the other disorder

strengths and the results confirmed, in the same way, the sufficiency of the number of random realizations. We also note that the simulations were performed on an HPC center with Intel Xeon Gold 6148 processors at 2.40 GHz and the longest run time lasted approximately six hours for a single parameter set and random realization.

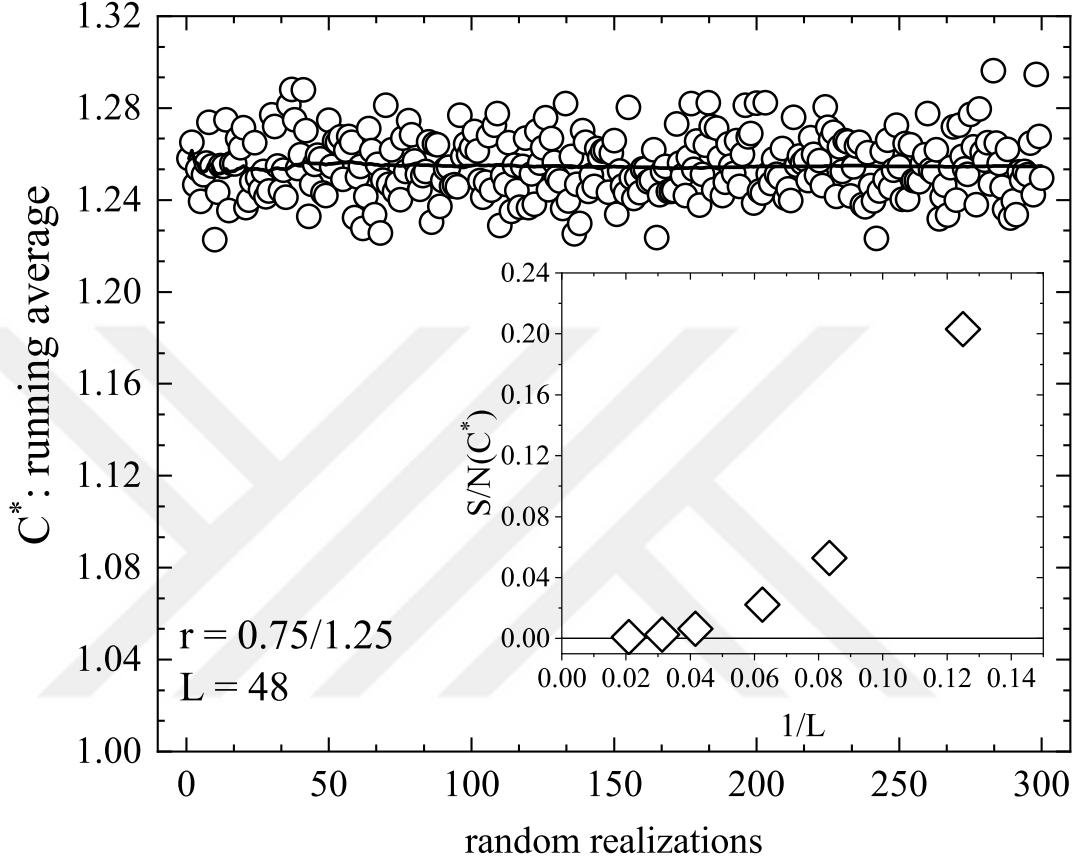


Figure 4.1 Specific heat values (empty circles) and the running average (solid line) of each disorder realization near the critical temperature for $L = 48$ and $r = 0.5/1.5$. The inset shows the signal to noise ratio (S/N) of the specific heat according to inverse system sizes

We use the estimators that are given in the preceding chapters to calculate the averages of quantities of interest. We use Eq. (2.36) for the specific heat, C , estimator and Eq. (2.66) for the staggered susceptibility, $\chi_s(\mathbf{Q})$, estimator, where $\mathbf{Q} = (\pi, \pi, \pi)$ is the 3D ordering wave vector. We use Binder ratios and the spin stiffness as dimensionless quantities to obtain the critical points and the exponents. Binder parameters are derived from the ratios of magnetization moments,

$$R_1 = \frac{\langle (m_s^z)^2 \rangle}{\langle |m_s^z| \rangle^2} \quad (4.1a)$$

$$R_2 = \frac{\langle (m_s^z)^4 \rangle}{\langle (m_s^z)^2 \rangle^2} \quad (4.1b)$$

and the spin stiffness is calculated for all spatial dimensions and averaged,

$$\rho_s = \frac{1}{3\beta} \sum_{\alpha=x,y,z} \langle W_\alpha^2 \rangle \quad (4.2)$$

where $W_\alpha = \frac{1}{L} [\mathcal{N}_\alpha(+)-\mathcal{N}_\alpha(-)]$ is the winding number as defined in Eq. (2.73).

In the next section, crossing point analyses are used to get the critical points and the exponent so the propagated data will be highly correlated. Thus for statistically sound fits, the full covariance matrix should be taken into account. The errors of the propagated data were calculated by using the bootstrap resampling method and a thousand bootstrap blocks were generated for the quantities R_1 , R_2 , and $L\rho_s$. Let V be a matrix of deviations per block generated from the intersections (either the intersections themselves or functions of intersections) of a quantity. Then the covariance matrix is defined as

$$C = V^T V \quad (4.3)$$

and from which the chi-square (χ^2) value of a fit can be calculated as in the following

$$\chi^2 = u^T (C^{-1}) u \quad (4.4)$$

where u is a column matrix of the deviations of the estimated intersections (or their functions) from the corresponding values of the fit function. It should be noted that in the statistical analysis conducted here there are two sources of random errors, one from the MC simulations and the other is due to the bootstrap resampling. The final effect of this is to reduce the chi-square by half. The goodness of fit is determined by the average chi-square per degree of freedom which is expected close to one, i.e., $\langle \chi^2/N_d \rangle \approx 1$. The standard deviation of $\langle \chi^2/N_d \rangle$ is $\sqrt{2/N_d}$ and our goodness of fit results deviate from the expected value at most one or two standard deviations.

4.2 Results and Discussion

We calculate the T_N for each disorder strength using spin stiffness and the Binder ratios. Hyperscaling theory gives the FSS form of the spin stiffness as $\rho \propto L^{2-d-z}$ in the vicinity of the phase transition point (Wallin et al., 1994). Here d is the dimension of the system and z is the dynamical critical exponent which is zero for finite-temperature phase transitions. This means that ρL is independent of the system size at the critical (Néel) temperature. The variations of R_1 and R_2 at the temperatures near the critical point are shown in Figure 4.2 and Figure 4.3 for selected system sizes, respectively.

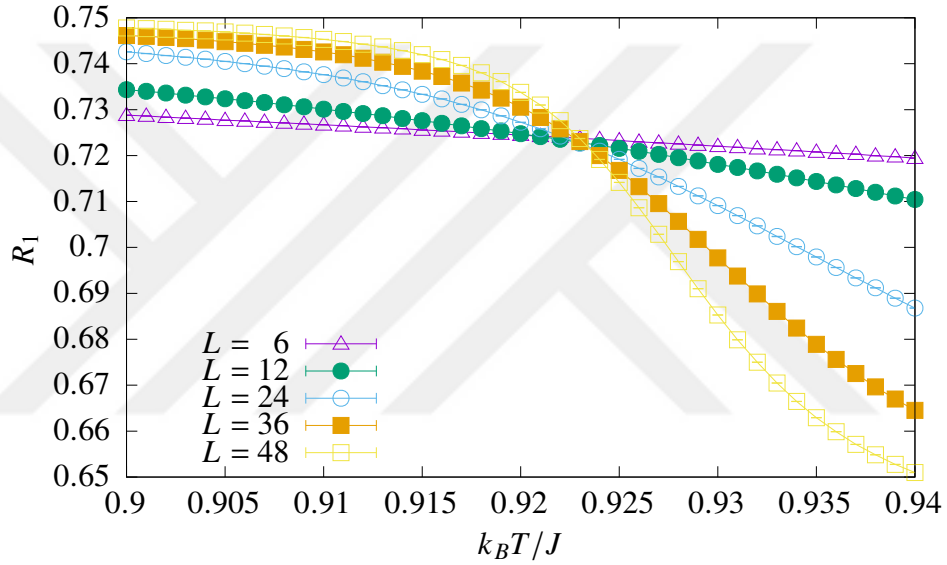


Figure 4.2 Temperature dependence of R_1 near the critical point for selected system sizes. The lines are guides to the eye

The curves of different system sizes cross each other systematically near the phase transition point. Similar behavior is also present for the spin stiffness ($L\rho_s$) curves that are shown in Figure 4.4 for the same selected system sizes. The pattern of the intersections can best be unveiled by making crossing point analysis with a selected aspect ratio of the system size couples. The intersection points shift to the critical point either from left or right depending on the quantity. Here we select the couples as $(L, 2L)$ among all the system sizes available. The crossing point of the couples is determined by performing a polynomial interpolation to the data near the intersection. In Figure 4.5 we see values of R_2 near the intersection of couples for the selected system

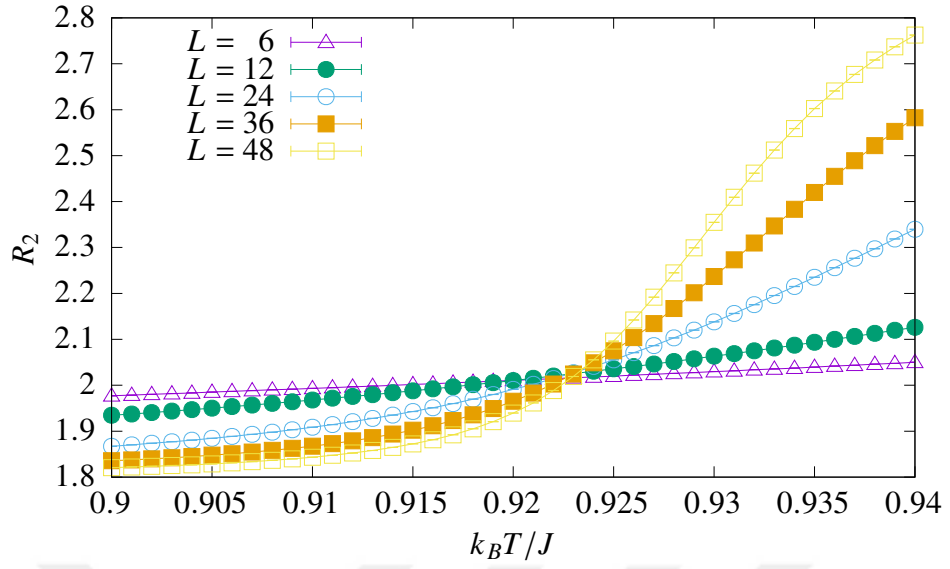


Figure 4.3 Temperature dependence of R_2 near the critical point for selected system sizes. The lines are guides to the eye

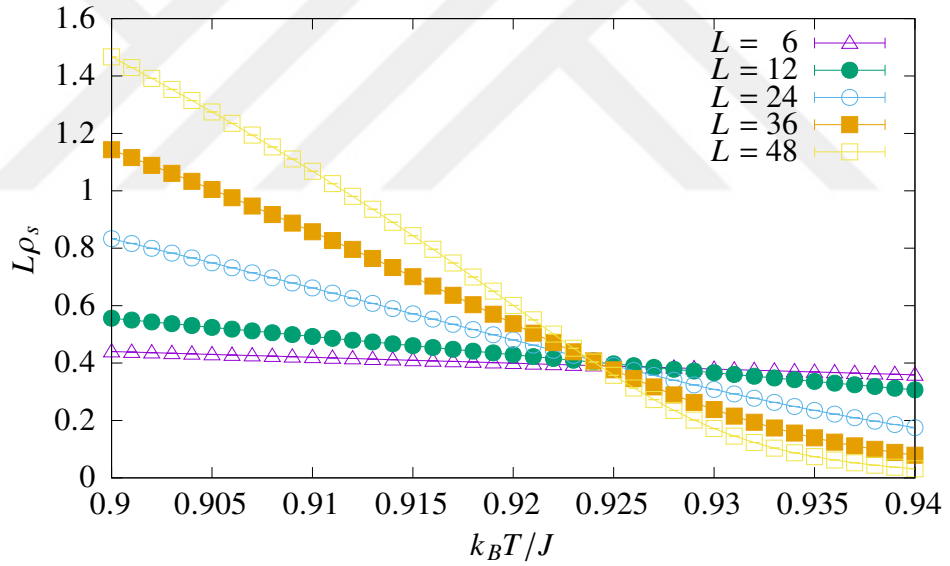


Figure 4.4 Temperature dependence of $L\rho_s$ near the critical point for selected system sizes. The lines are guides to the eye

sizes. The crossing point of a selected couple $(L, 2L)$ is the root of the differences of the corresponding polynomials. This root can be found by numerical methods such as bisection or Newton. Those procedures are repeated for the other quantities (R_1 and $L\rho_s$) and parameters ($r = 0.9/1.1, 0.5/1.5$) as well.

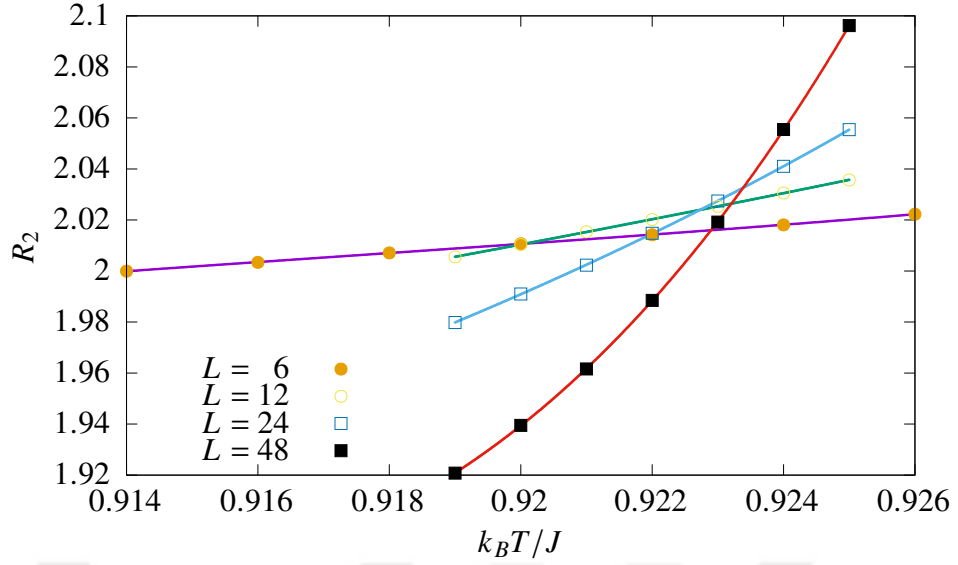


Figure 4.5 R_2 values near the intersection points of the couples $(L, 2L)$ for selected system sizes. The solid curves are cubic polynomial fits to data. The error bars are smaller than the data points

Next, we fit the data extracted from crossing point analysis to the expected forms. We exclude the smallest system size until we get a statistically sound fit based on the criterion

$$\frac{\chi^2}{N_d} < 1 + 2\sqrt{\frac{2}{N_d}} \quad (4.5)$$

in which we tolerated up to two standard deviations at most from the expected average chi-square per degree value. The crossing points generated from R_1 , R_2 , and $L\rho_s$ couples were fitted separately to Eq. (1.22) with $g_L = T_L$ and $g_c = T_N$ as shown in Figure 4.6. The fits start to satisfy the condition in Eq. (4.5) for R_1 with sizes $L \geq 6$, for R_2 with sizes $L \geq 8$, and for $L\rho_s$ with sizes $L \geq 10$ and the corresponding χ^2/N_d values are 0.32, 1.13, and 1.23, respectively. The extrapolated infinite size critical temperature is estimated as $T_N = 0.92363(3)$. It is clear in Figure 4.6 that the intersection points of the size couples get close to T_N from the left for Binder ratios and from the right for spin stiffness. We obtain the critical temperatures for other disorder strengths using the same procedures to be $T_N = 0.94075(3)$ and $T_N = 0.86161(1)$ for $r = 0.9/1.1$ and $r = 0.5/1.5$, respectively.

Now we calculate the correlation length critical exponent ν from the data of R_2 by using Eq. (1.24) (with $Q = R_2$) and the critical temperatures found above. The

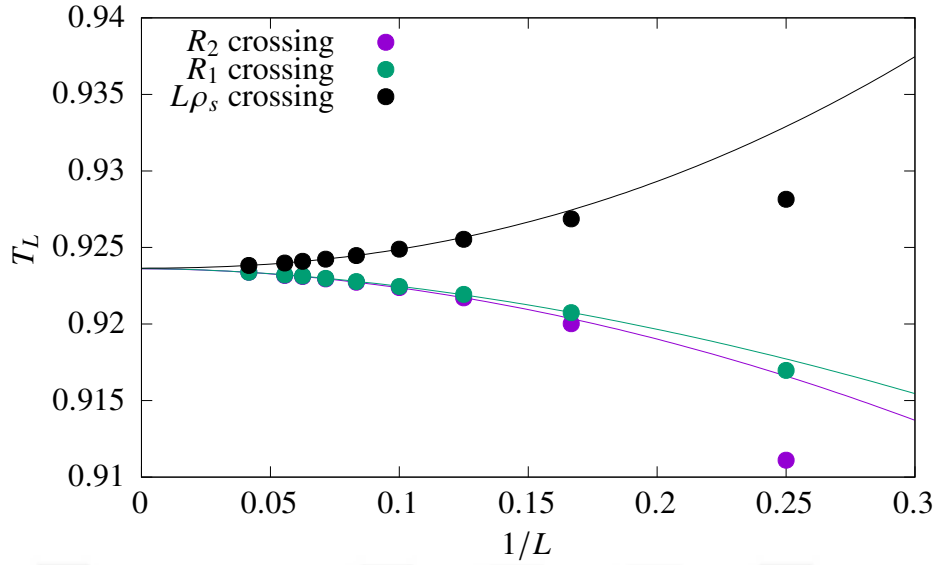


Figure 4.6 Crossing temperatures of Binder ratios and the spin stiffness for all couples versus $1/L$. The curves are fits to Eq. (1.22). The error bars are smaller than the data points

derivative of R_2 is taken at the critical temperature T_N after making cubic polynomial interpolations to data near the critical temperature for each system size L . The power-law fit to extract ν is shown in Figure 4.7 and the value of the critical exponent is found to be $\nu = 0.705(2)$. The fit in Figure 4.7 is performed for system sizes $L \geq 6$ and the corresponding chi-square per degree is $\chi^2/N_d = 0.21$. The critical exponent is estimated as $\nu = 0.706(7)$ and $0.709(7)$ for the disorder parameters $r = 0.9/1.1$ and $0.5/1.5$, respectively. Those findings up to now can convince one that the disordered model investigated here is in the 3D classical Heisenberg universality class.

We also estimate the critical exponent ν directly from the Eq. (1.27) without the need to know the critical temperature. For this, we use spin stiffness data $L\rho_s$ and calculate the crossing points and the derivatives at those points by using cubic interpolations as before. The left-hand side of Eq. (1.27) (with $Q = L\rho_s$) can be regarded as an exponent estimate for the finite-size system (or for the crossing point) so it is defined as $1/\nu_L$. The calculated results together with the fit are shown in Figure 4.8 where all system sizes ($L \geq 4$) are included in the fit. The fit looks statistically sound despite the noisy data and the large error bars at smaller system sizes. The extracted exponent is the same as calculated above, namely, we found $\nu = 0.705(6)$.

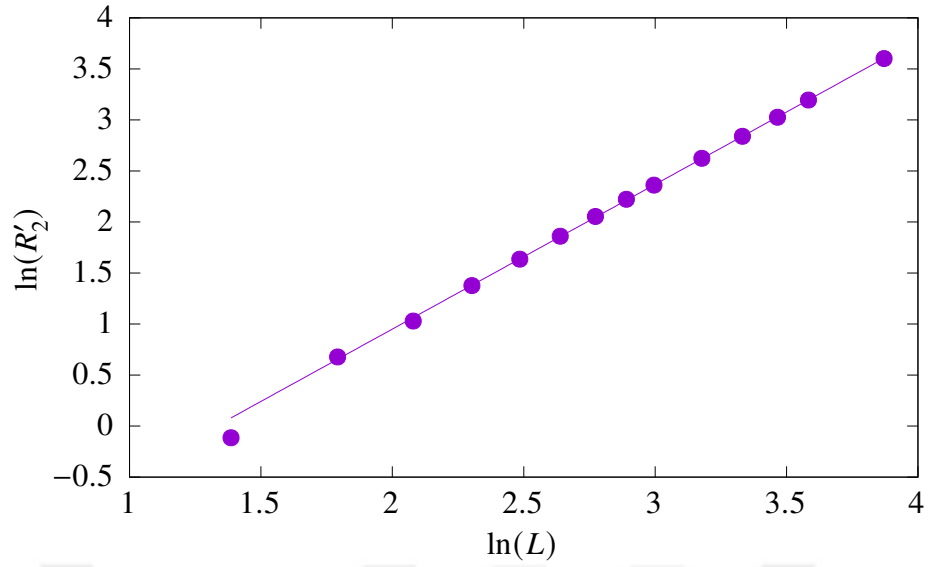


Figure 4.7 The points are the logarithms of the derivatives of R_2 at the critical temperature versus $\ln(L)$. The line is a fit ($L \geq 6$) to Eq. (1.24). The error bars are smaller than the data points

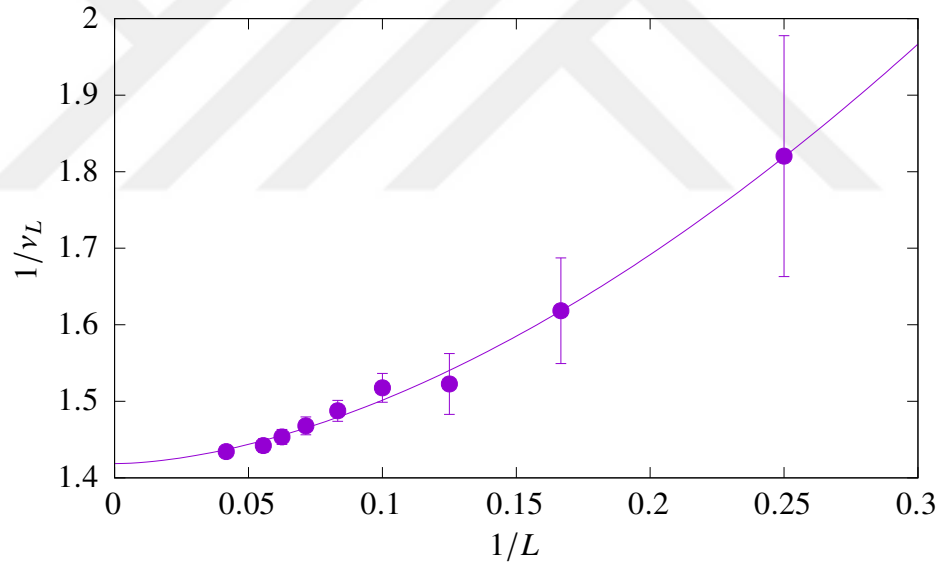


Figure 4.8 The points are the estimated inverse correlation length exponent of the system calculated from the left-hand side of the Eq. (1.27) with spin stiffness data ($L\rho_s$). The curve is a fit to Eq. (1.27) at all system sizes ($L \geq 4$)

Having determined the critical temperature (T_N) and the critical exponent of the correlation length (ν), the critical exponents of the magnetization (β) and staggered susceptibility (γ) can be calculated. For this, we use Eq. (1.20) with $\kappa = \beta, \gamma$ by

discarding the leading correction term thus we have,

$$Q(\delta, L) \propto L^{\kappa/\nu} \quad (4.6)$$

where we use $\langle |m_s^z| \rangle$ and $\chi_s(Q)$ for $Q(\delta, L)$ to calculate the exponents β and γ , respectively. Figure 4.9 shows the logarithm of the calculated estimate $\langle |m_s^z| \rangle$ for each system size and a linear fit in the form of the logarithm of the Eq. (4.6) from which the exponent ratio is calculated to be $\beta/\nu = 0.518(2)$ as the slope of the fit line.

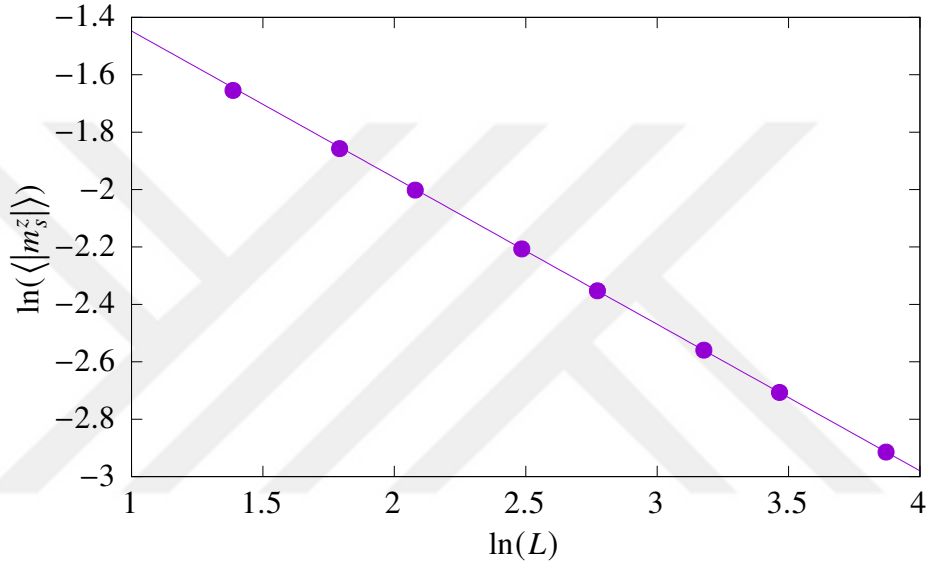


Figure 4.9 The points are the logarithms of the estimated absolute value of the staggered magnetization versus $\ln(L)$. The line is a fit to the Eq. (4.6) with $\kappa = \beta$ and $Q = \langle |m_s^z| \rangle$ at system sizes $L \geq 12$. The ratio of critical exponent $\beta/\nu = 0.518(2)$ is the slope of the fit line. The error bars are smaller than the data points

Similarly, Figure 4.10 shows the logarithm of the estimated staggered susceptibility $\chi_s(Q)$ for all system sizes and the fit line from the points $L \geq 12$ to the form of Eq. (4.6). The slope of the fit line gives the exponent ratio $\gamma/\nu = 1.962(5)$. Now we are in a position to test the calculated critical values within a single equation. By leaving the leading correction term out in Eq. (1.20) and sketch $\delta L^{1/\nu}$ (with $\delta = T - T_N$) versus $Q(\delta, L)L^{-\kappa/\nu}$ we expect the data to collapse onto a single curve at system sizes large enough. Here we use staggered susceptibility data, i.e., $Q = \chi_s$ and $\kappa = \gamma$ to check the expected collapse. Figure 4.11 shows the data points sit on the same curve as expected for system sizes $L \geq 12$.

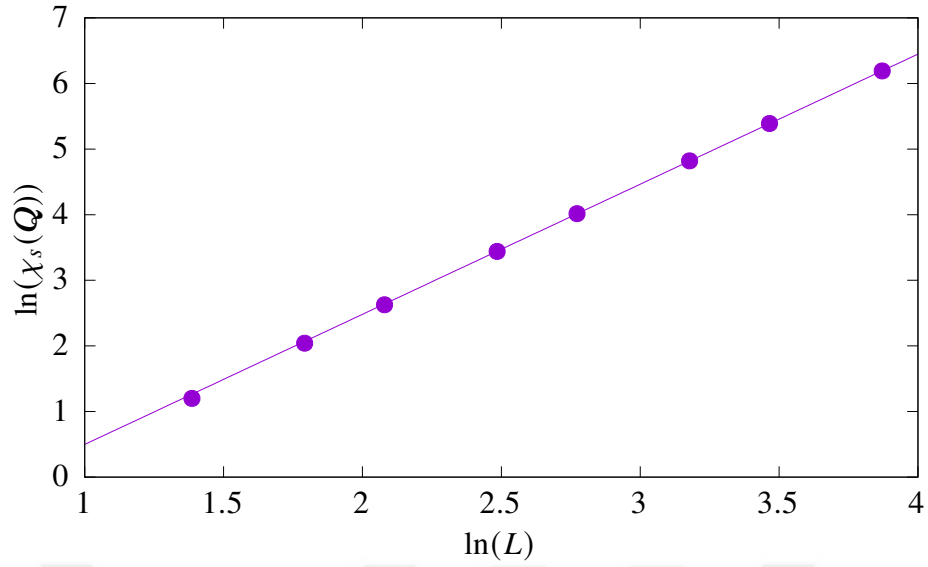


Figure 4.10 The points are the logarithms of the estimated staggered susceptibility versus $\ln(L)$. The line is a fit to the Eq. (4.6) with $\kappa = \gamma$ and $Q = \chi_s(Q)$ at system sizes $L \geq 12$. The ratio of critical exponents $\gamma/\nu = 1.962(5)$ is the slope of the fit line. The error bars are smaller than the data points

The remaining system sizes do not match with the curve due to the neglected correction term for which we didn't attempt to extract the critical exponent. Here the values of the critical temperature and the correlation length exponent can be regarded as the correct values of the infinite size system because their estimation steps include the scaling correction term at the first order. However, in the estimation of the critical exponents β and γ the correction terms are completely ignored. Nevertheless, the results up to now are enough to say that the 3D quantum Heisenberg model with bimodal disorders is in the universality class of the classical Heisenberg model.

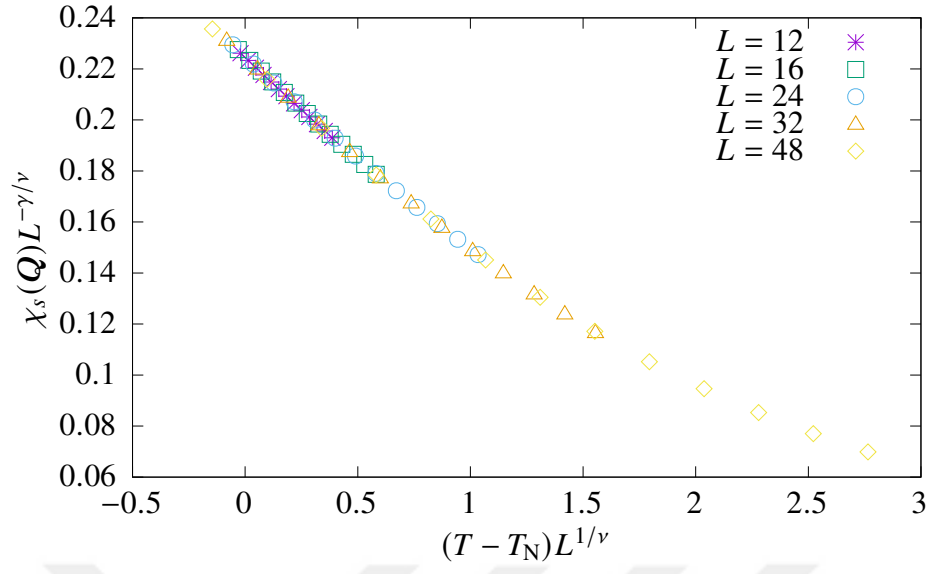


Figure 4.11 The points are the scaled data for the staggered susceptibility by using the extracted critical values, $T_N = 0.9236$, $\nu = 0.705$, and $\gamma/\nu = 1.962$. The data collapse onto the single curve for the system sizes $L \geq 12$

CHAPTER FIVE

SUMMARY AND CONCLUSIONS

The quantum spin systems exhibit fascinating properties compared to their simple definition, as we experienced in the preceding chapters. This is mostly due to the deep connection to the Pauli mechanism via the Heisenberg-like models that account for the exchange interactions implicitly. Spin systems have successfully described the critical phenomena and universal behavior so far in magnetic materials. Phase transitions of real materials are mimicked by spin models and RG theory enables FSS analysis of MC simulations as well as theoretical calculations. Dealing with the dimensional (both spin and spatial) complexity of spin systems has been a major problem of condensed matter physics. The modern computers of today even the most powerful HPC centers are very far away from the required resources for the exact numerical treatment of a system large enough to get real physical results.

Actually it should have not been necessary to account majority of the terms of the partition function and the researchers found a way of approaching a physical system with computers as nature does. The random or fluctuating property of MC logic mimics the behavior of a system that is in equilibrium in a bath. It is not a surprise but a breakthrough that the Metropolis algorithm was proposed nearly at the same time as the invention of computers. In time the MC methods have evolved to the modern form today used. The modern forms of MC methods are just more efficient than their primitive counterparts. Any MC method either with local or global updating will yield the correct sampling if we wait an infinite time. This is the power of MC methods they don't suffer dimensionality problems provided that we wait enough time. Although the modern QMC methods are so efficient they still suffer from the infamous sign problem as a surprise. As mentioned before this not a deficit of the method but a restriction to varieties of models to apply. The disorder in a system does not limit the applicability of MC simulations, in contrast the self-averaging property makes the system to be treated as a quenched one as in the case of a laboratory experiment on a sample. Thus one can easily simulate the disordered systems just if there are enough processors.

The Metropolis algorithm is still at the heart of most (Q)MC techniques. Years after the proposition of the Metropolis algorithm RG theory came to the scene and put the FSS analysis on the rigorous ground. Now the modern SSE technique is well suited for simulating quantum spin systems, it is versatile and handy to implement, as we saw. SSE technique is based on the Taylor series expansion of the partition function differently than a Trotter decomposition in the conventional PIMC method. So it does not include any approximation stemming from the definition of the algorithm. The efficiency of the SSE technique is closely related to the discrete representation of the quantum partition function. Non-diagonal operators such as specific heat and staggered susceptibility can efficiently be measured. For the special cases, exemplified in the previous chapters, the SSE technique can be implemented with deterministic loops that make the simulation more efficient for certain models. A bond-represented formalism implements the algorithm easily to different geometries, just by arranging bonds between the spins. Test calculations compared with the ED results showed the SSE technique gives exact results up to desired precision. The precision of the results depends on the run time of the SSE algorithm i.e. the number of data groups collected. Using the spin half isotropic Heisenberg model as a test model is a good starting point to get the basic ideas of a QMC method and extend it to more general class models.

As a result, we applied the SSE QMC technique to a ladder model and a 3D model (Kanbur, Polat, et al., 2020). The SSE QMC method was used to study the thermal and low-temperature properties of a two-leg ladder system with a bimodal disorder along its rungs. For the quantities specific heat and the uniform susceptibility, we found special temperature points, separately, at which the results are independent of the disorder strength. The results corresponding to those crossing point values can belong to a class of models exhibiting a nearly universal behavior. The physical outcomes are not so different from the clean case. This can be linked to the interaction types of the bonds that are the same for the whole system. The decreasing property of the spin gaps is also present in the clean system with decreasing rung couplings. But here the smallest gap value is well above the weak coupling limit of the clean system. As a final word, the properties of a two-leg ladder system with disorder only along the legs or along both directions might be interesting. As the Hubbard model with half-filling and the

Heisenberg model are equivalent, the exact or approximate values for the crossing points can be calculated theoretically.

The effects of the quenched disorder on the critical properties of the 3D Heisenberg antiferromagnetic model are explored in the preceding chapter (Kanbur, Vatansever, et al., 2020). Large-scale SSE QMC simulations were performed for the system sizes up to $L = 48$ ($N = L^3$ sites). Systematic crossing point analysis was made by using separately the intersections of the quantities R_1 , R_2 , and $L\rho_s$ and estimated the critical values for all disorder parameters by FSS procedures applied to crossing points. The critical exponent ν was estimated using estimated critical temperature and directly without any critical value. For all disorder strengths, the result for the critical exponent ν from the two analyses was found to be the same within statistical errors and it is the universal value of the 3D classical Heisenberg universality. Thus we conclude that the universal behavior of the model considered here is independent of the disorder included among the spin interactions. An important concept we touched on in the first chapter is the stability of the clean system against a disorder can be tested with the Harris criterion. For our results, the condition $d\nu > 2$ is satisfied and the Harris criterion is not violated.

We should emphasize the importance of the systematic FSS analysis conducted in the fourth chapter. It is very important to take into account the covariance matrix of the correlated data for a statistically correct analysis. The crossing points arising from different system sizes are highly correlated. The other important concept in the error analysis is the bootstrap resampling method. While the bootstrap methods have been controversial among the statisticians after its development by Efron (1979), it is widely used in statistical analysis (Press, 1996).

One final consideration is that for models with large diagonal terms (e.g., bosonic Hubbard models) or with time-dependent actions (e.g., dissipative quantum systems) the PIMC technique could be preferred. The reason is that in the PIMC technique the diagonal terms are treated exactly and only the off-diagonal terms are perturbed. In other words, the SSE QMC technique treats both diagonal and off-diagonal terms perturbatively. Although the expansion in the PIMC method needs few terms, one

has to deal with imaginary times. In the quantum spin systems, the diagonal and the off-diagonal terms are mostly well balanced. As a result, the discrete representation of the SSE QMC method and its versatile implementation make it an expedient technique for simulating quantum spin systems at either zero or finite temperatures.



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