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Data Accuracy Dependence on Number of Bins in Stochastic Series Expansion for Spin-1/2 Antiferromagnetic Heisenberg Chains

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ABSTRACT

Background:

Antiferromagnetic systems exhibit complex quantum behaviours that require accurate numerical methods to analyse. The Stochastic Series Expansion (SSE) is a quantum Monte Carlo technique that simulates these systems. This study examines the effect of the number of bins on the accuracy of physical property measurements using SSE.

Materials and Methods:

The SSE simulations were performed using Fortran 90 on a Ryzen 7 processor. The system was initialised with varying lattice sizes (64, 128, 256, and 1024) and dimensionless temperatures (1/32, 1/16, 1/2, and 4) to analyse different configurations. N_{bins} and Monte Carlo steps were adjusted systematically to investigate their impact on the results. Results were visualised in Origin Lab.

Results:

Increasing the number of bins (N_{bins}) reduced fluctuations, leading to reliable results, especially at low temperatures. Lower temperatures lead to higher fluctuations in susceptibility and specific heat of the system. The Neel temperatures were observed around dimensionless temperature. $T/J = 0.5$ Indicating phase transitions.

Conclusions:

The study shows that N_{bins} are crucial for accurate results in SSE simulations. Although the method is effective for most properties, specific heat calculations require higher computational costs and present limitations in precision.

Keywords: Linear chain; Stochastic series expansion; Spin-1/2; Antiferromagnetic; Quantum Monte Carlo.

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INTRODUCTION

Today, Stochastic Series Expansion (SSE) is a standard tool for studying quantum magnetism, phase transitions, and low-dimensional systems due to its efficiency in simulating both ground state and finite-temperature properties of quantum systems. The SSE method is a Quantum Monte Carlo (QMC) algorithm that simulates quantum spin and bosonic systems. QMC methods numerically solve many-body problems that are difficult or impossible to solve analytically. QMC methods map the quantum system onto a classical one to make them suitable for applying classical Monte Carlo techniques[1-3].

The SSE origins date back to the 1960s when D. C. Handscomb suggested expanding the partition function into a series representation. The method was inefficient for practical computations because it resulted in slow convergence and high computational cost. But in the 1990s, Andres W. Sandvik improved the technique by developing an update scheme using a loop algorithm. This modification allowed SSE to handle larger system sizes and longer simulation times with reduced computational cost. SSE can handle the partition function directly using a series expansion. This technique avoids the sign problem that appears in other QMC algorithms, making it an essential tool for studying a wide range of magnetic materials with complex interactions [4-6].

Antiferromagnetic materials are a class of magnetic systems in which the spins of adjacent atoms are aligned in opposite directions, leading to zero net magnetization. These materials are crucial in many technological applications, such as spintronics and magnetic storage devices. Studying these systems enhances understanding of strongly correlated systems and quantum phase transitions. The Heisenberg model, which describes the interaction between spins on a lattice, is essential in simulating an antiferromagnetic system and capturing the exchange interaction between neighboring spins. This model enables the study of anisotropy in spin interactions, bringing the simulation closer to the thermodynamic behavior of real antiferromagnetic materials [7-11]. **Figure 1** shows a schematic diagram of the magnetic ordering of an antiferromagnetic material.

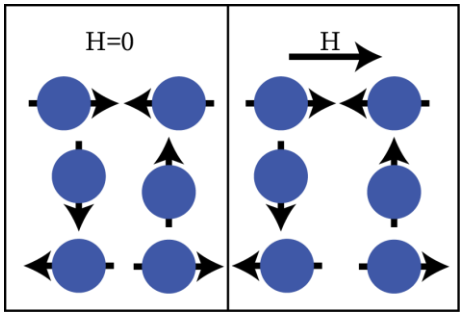

Figure 1: Antiferromagnetic ordering in the material where adjacent spins align in opposite directions.

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The SSE accurately estimates the physical quantities of the system, such as ground state energy, specific heat, susceptibility, and sub lattice magnetization. It efficiently samples the partition function using a series of diagonal and off-diagonal operators. One crucial property emerging from studying antiferromagnetic systems is the Néel temperature, the critical temperature below which long-range antiferromagnetic order sets in. Above this temperature, thermal fluctuations dominate, destroying the magnetic order, while below it, the spins align in an alternating pattern, leading to a stable antiferromagnetic phase [12,13].

The accuracy and stability of results in the SSE simulations depend on several parameters that must be optimised to obtain reliable results. The essential parameters include equilibration steps, Measurement steps, and the N_{bins}. The Monte Carlo step is the basic unit of the SSE simulation; it involves proposing updates to the spin configuration according to probabilistic criteria (typically the Metropolis algorithm). These updates either act on the local spin configuration without changing the spin state (diagonal update) or flip the spins to a different state (off-diagonal update). Equilibration steps (I_{steps}) are Monte Carlo steps performed at the beginning of the simulation to bring the system into a thermal equilibrium state. In this stage, no measurements of physical properties are taken. If the number of equilibration steps is insufficient, the results will be biased, leading to inaccurate physical properties. After equilibration, measurement sweeps (MC Sweeps) are performed to measure the system's physical properties, such as energy, magnetization, susceptibility, and specific heat are recorded. The measurement sweeps are repeated to obtain an accurate average. N_{bins} represents how many independent averages are taken during the simulation. Each bin contains the average results from several measurement sweeps. Averaging over all the bins gives the final estimate of the physical properties [14,15].

This paper aims to study and analyse the results of the SSE methods in terms of N_{bins} and their effect on measuring the physical properties of a specific system at low temperatures and relatively large sizes.

THEORETICAL BASIS OF THE STOCHASTIC SERIES EXPANSION (SSE)

The key idea behind the SSE approach is to express the partition function as a power series expansion of the Hamiltonian based on diagonal and off-diagonal operators [16].

- **Partition Function in the SSE Formalism**

The starting point is the partition function, which is defined as:

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right], \qquad (1)$$

where $\beta = \mathrm{J}/T$ is the inverse dimensionless temperature where J is the exchange interaction constant, T is the temperature and H is the Hamiltonian of the system. This representation normalizes the temperatures relative to the energy scale of the system, making β unitless, thereby simplifying the analysis of thermodynamic properties. In the SSE, the partition function is rewritten using a Taylor series expansion [17]:

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$$Z = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \mathrm{Tr}[(-H)^n] \quad (2)$$

For a typical spin-1/2 Heisenberg model, the Hamiltonian is given by [18]:

$$H = -J \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ + \Delta S_i^z S_j^z \right) \quad (3)$$

where J is the exchange interaction constant, Δ is the anisotropy parameter, $S_i^{\pm}$are the spin raising and lowering operators and S_i^z is the spin-z component operator. The summation $\langle i,j \rangle$ runs over all nearest neighbor pairs in the lattice.

- **Operator String Representation**

The SSE formalism maps the power series of H onto a series of discrete operators. The Hamiltonian is decomposed into local bond Hamiltonians [19]:

$$H = \sum_b H_b \quad (4)$$

where H_b acts on a pair of spins connected by a bond b. Each H_b can be further split into diagonal (H_b^d) and off-diagonal (H_b^o) parts. An operator string represents the power series expansion in the SSE method $S = [H_{b_1}, H_{b_2}, \dots, H_{b_n}]$ and a corresponding spin configuration $|\alpha\rangle$ in the basis of the S^z-components of each spin.

The partition function is then written as [20]:

$$Z = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{S_n} \langle \alpha | (-H_{b_1})(-H_{b_2}) \dots (-H_{b_n}) | \alpha \rangle \quad (5)$$

where S_n denotes a sequence of n operators acting on the initial spin configuration $|\alpha\rangle$. The SSE method samples configurations of the operator string and spin states using Monte Carlo techniques. The update schemes include diagonal updates that change the length of the operator string and cluster updates that switch between diagonal and off-diagonal operators. Once equilibrium is reached, properties can be measured using the sampled configurations.

- **Metropolis-Hasting algorithm**

The Metropolis-Hasting algorithm is a method for sampling from a probability distribution. The algorithm starts with an initial state (θ^0) then proposes a new state (θ') from the distribution $q(\theta'|\theta)$ wich gives a candidate state (θ') using the current satate (θ). The Metropolis algorithm calculates the acceptance probability (α) using the formula [21]:

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$$\alpha = min\left(1, \frac{P(\theta')q(\theta \mid \theta')}{P(\theta)q(\theta' \mid \theta)}\right) \quad (6)$$

Where: $P(\theta)$ is the probability of the current state, $P(\theta')$ is the probability of the proposed state, $q(\theta' \mid \theta)$ is the probability of proposing θ' from θ, and $q(\theta \mid \theta')$ is the reverse proposal probability. The algorithm generates a random number $u \in [0,1]$. If $u \leq \alpha$, accept θ' and set $\theta = \theta'$. however, if $u > \alpha$, reject θ' and retain θ [22], [23]. **Figure 2** shows that the algorithm starts from an initial sample θ^0 and generates a sequence of samples by proposing new states θ' using a prior distribution $p(\theta)$. Each proposed state is either accepted or rejected based on the acceptance probability, guiding the chain to areas of higher probability density. The figure shows accepted moves (solid lines) and rejected moves (dashed lines). After sufficient iterations, the sampled distribution converges to the desired posterior distribution $P(\theta \mid y)$, reflecting the underlying probability distribution

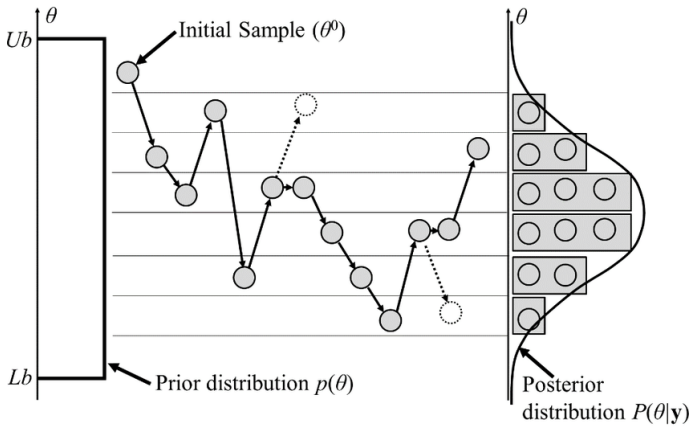

Figure 2: Illustration of the Metropolis-Hastings Sampling Process[24].

- **Calculation of Physical Properties Using the SSE**

The SSE method allows for the direct calculation of various thermodynamic quantities. The key observables include the ground state energy, specific heat, magnetic susceptibility, and sublattice magnetization.

a) Ground State Energy:

The ground state energy per site is obtained from the expectation value of the Hamiltonian [25], [26]:

$$E = \frac{1}{\beta}\langle n \rangle \quad (7)$$

where n is the expansion order of the series, and $\langle n \rangle$ is its Monte Carlo average. The expression arises because the partition function Z is proportional to β^n.

b) Specific Heat:

The specific heat C is calculated from the fluctuation of the energy [27]:

$$C = \frac{\langle n^2 \rangle - \langle n \rangle^2}{N k_B T^2} \tag{8}$$

where N is the total number of spins in the system, and $\langle n^2 \rangle$ is the variance of the expansion order.

c) Magnetic Susceptibility:

The magnetic susceptibility χ measures the response of the system to an external magnetic field and is given by [28]:

$$\chi = \frac{\beta}{N} \left\langle \left(\sum_i S_i^z \right)^2 \right\rangle \tag{9}$$

where $\sum_i S_i^z$ is the total magnetization along the z-axis.

d) Sublattice Magnetization:

For antiferromagnetic systems, the sub lattice magnetization is an important order parameter, defined as [29]:

$$\langle m^2 \rangle = \frac{1}{N} \left\langle \left| \sum_{i \in A} S_i^z - \sum_{j \in B} S_j^z \right| \right\rangle \tag{10}$$

where A and B denote the two sublattices of the system. This quantity indicates the degree of local ordering within the antiferromagnetic phase.

MATERIALS AND METHODS

The SSE simulation was performed on a computer with a Ryzen 7 3700x processor and 16 GB of RAM. The simulation code was implemented in Fortran 90 following the Sandvik algorithm. Data analysis was conducted using IBM SPSS, while visualization was carried out using Origin Lab 2024b. Microsoft Excel 2021 was used for data organization.

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The SSE code begins by initializing key parameters such as lattice dimensions, inverse temperature, and Monte Carlo steps. The lattice structure is defined based on system size and boundary conditions, and a random number generator is initialized for stochastic sampling [30]. The simulation consists of two main phases: Equilibration and Measurement. During equilibration, a specified number of Monte Carlo steps is used to update the system until it reaches thermal equilibrium. This is achieved using diagonal and loop updates to ensure the system accurately represents equilibrium properties. The process of one Monte Carlo step is represented in **Figure 3**. The Metropolis algorithm is used in the diagonal update subroutine of the SSE code. When a new configuration is proposed by either adding or removing diagonal and off-diagonal operators. The acceptance and reflection of this configuration follow the Metropolis criterion [31].

In the measurement phase, a series of Monte Carlo sweeps (MC Sweeps) is performed to calculate physical properties such as energy, specific heat, magnetization, and susceptibility. These values are averaged over several bins (N_{bins}) to improve statistical accuracy. Dynamic cutoff adjustments handle any increase in operator string length; final results are written to output files for analysis. The memory is deallocated at the end to ensure efficient resource management. This structured approach ensures accurate and reliable simulations of quantum spin systems.

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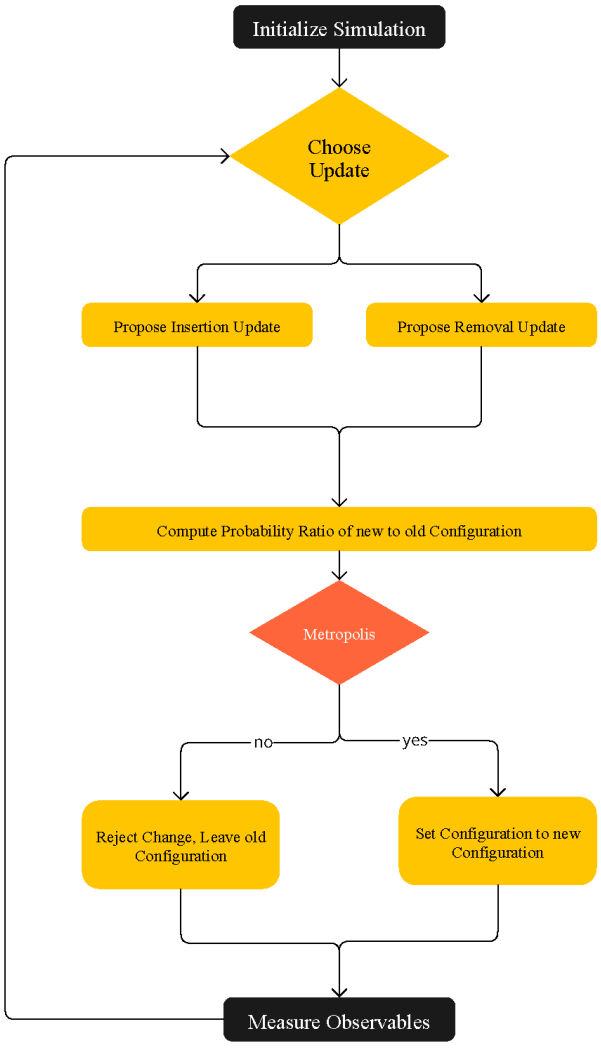

Figure 3: Schematic diagram of one Monte Carlo step in the simulation [32]**.**

RESULTS AND DISCUSSION

In this section, we present the results of the Stochastic Series Expansion (SSE) simulations for the 1D spin-1/2 Heisenberg antiferromagnetic model, focusing on the impact of binning and Monte Carlo sweeps on the accuracy of physical properties. We analyse the behavior of energy, specific heat, susceptibility, and sublattice magnetization across varying temperatures and system sizes to identify key trends and limitations.

- **Number of Bins**

Results show that the ground state energy remains stable across increasing N_{bins} for all beta values. Indicating good convergence and consistency in the results (See **Figure 4**), higher β (lower temperatures) result in lower ground state energies, which is consistent with the expected

behavioru of spin systems. The standard deviation (σ) increases with β decreases. Thermal effects on energy are more pronounced for higher temperatures. We can see that higher temperatures (lower β) result in high σ.

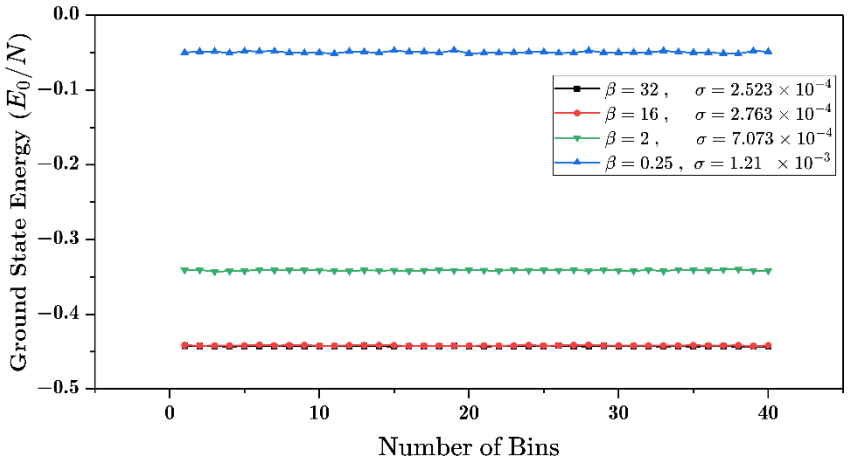

Figure 4: The relationship between the ground state energy and number of bins for different values of inverse dimensionless temperature ($\boldsymbol{\beta}$). Each point of this plot represented the average of energy across $\boldsymbol{MC\ sweeps = Isptes = 10^4}$ and for $\boldsymbol{Lx = 128}$. Where $\boldsymbol{\sigma}$ is the standard deviation of each dataset.

Figure 5 indicates that the results of $\langle m^2 \rangle$ are stable across increasing N_{bins} for all β values. Stronger magnetic ordering achived in higher values of β. The standard deviation is decreased for lower temperatures, thus resulting in higher precision.

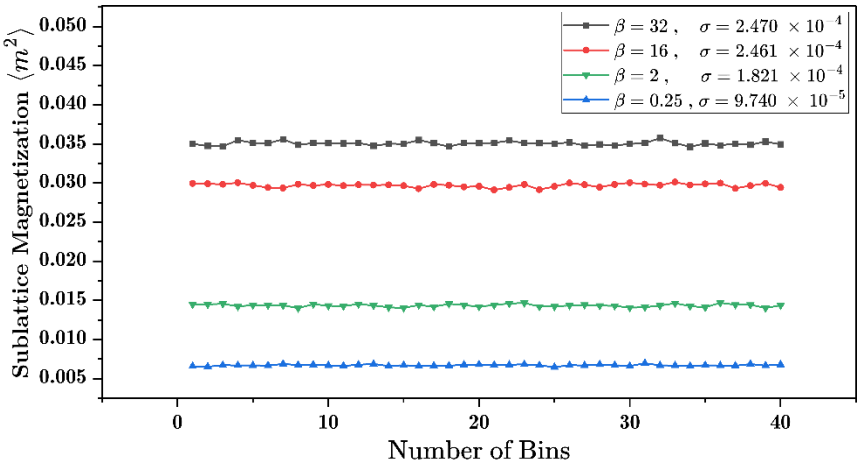

Figure 5: Variation of squared sublattice magnetisation with the number of bins for different $\boldsymbol{\beta}$. At lattice size $\boldsymbol{L_x = 128}$ and $\boldsymbol{MC\ sweeps = Isteps = 10^4}$. The standard deviation ($\boldsymbol{\sigma}$) is included in the legend.

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The values of χ are less stable than the ones from previous properties. We can notice from **Figure 6** that fluctuations vary significantly across different β values. The standard deviation values decrease with decreasing of β, meaning that lower temperatures yield more converge results. This behavior can ube explained by lower temperatures reducing thermal noise, and the quantum phenomena aominan ein lower temperatures. We can also notice from the figure that higher β values exhibit greater susceptibility as expected for antiferromagnetic systems; the magnetic ordering increases at low temperatures.

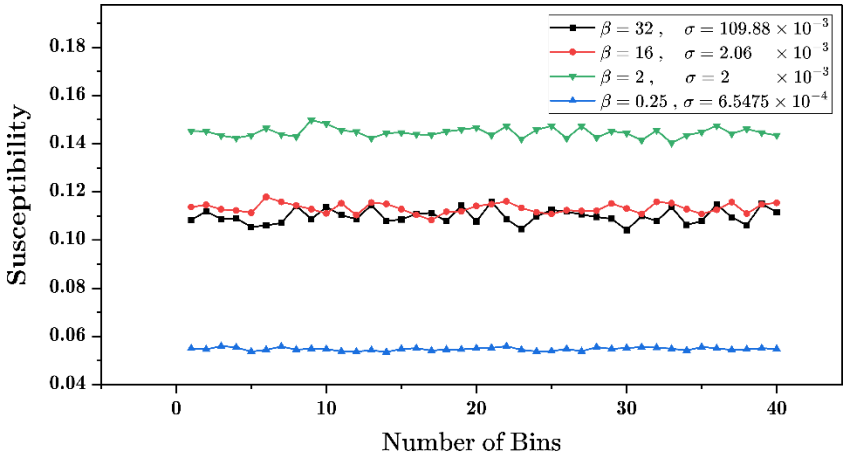

Figure 6: Susceptibility as a function of the number of bins across different β, for lattice size $L_x = 128$, and 10^4 of MC sweeps and I_{steps}. Higher accuracy of results is obtained from lower temperatures as represented by standard deviation (σ).

C pronounced oscillations for higher β values indicating poorly converged results as shown in **Figure 7**. This suggests that the system might require more I_{steps} or MC sweeps at lower temperatures to achieve reliable values. This can be marked as a drawback of the SSE in simulating the specific heat of low-temperature systems. As β decreases the fluctuation is reduced where $\beta = 0.25$ displaying the most stable outcomes. This aligns with the real systems; higher temperatures reduce the impact of quantum fluctuations. The presence of negative values in specific heat, especially at higher β, is almost vanishes after taking the average of all N_{bins}. However, this can indicate the need for more MC sweeps at each point and a sufficient value of equilibration steps.

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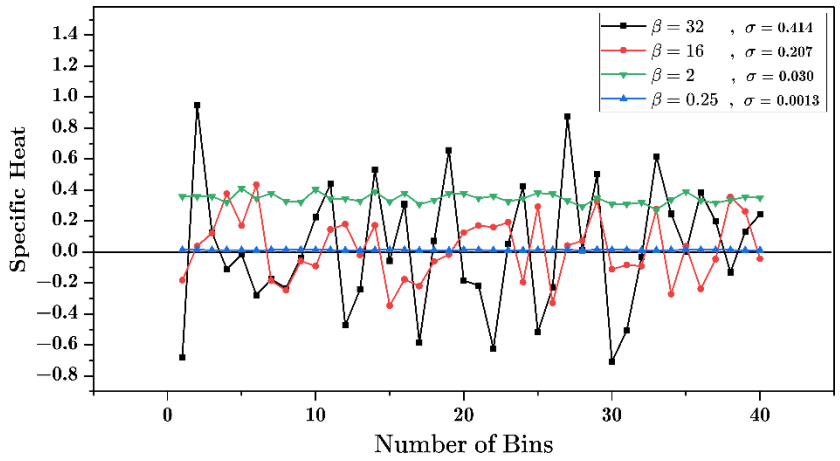

Figure 7: Specific heat results for across 40 bins for lattice size $L_x = 128$, and $Isteps = MC\ Sweeps = 10^4$. The simulation was conducted in different temperature conditions and the standard deviation of each condition's results is presented in the legend.

Neel Point Calculations

All the studied system sies exhibit a distinct peat at $T \approx 0.5$ which represnts the Neel temperature as shown in **Figure 8**. This peak indicates the transition from a disordered paramagnetic state to an ordered antiferromagnetic state as temperature is lowered. The main plot of the figure shows nearly equal curves of C is resulted from all the system sizes.and the peak become sharper with incresing of L_x; Thus more defined phase transition behavior of larger system.

The Comparison between solid and dotted lines shows little difference of results. Meaning that the results are well converged and the MC sweeps is sufficient in both state (10^4 and 10^6) in higher temperature. How ever lower temperatures showed a higher variability between solid and dotted lined as show in in **Figure 8**-b. The SSE uses random numbers in the simulation; thus the peak of specific heat is not one value, but a range of values that slightly differ from each other.

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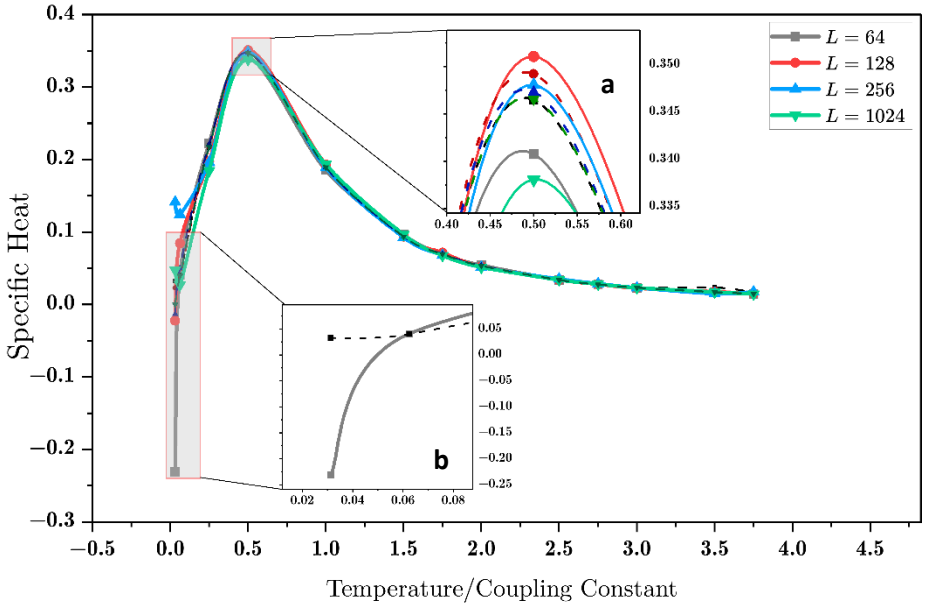

Figure 8: Temperature dependence of specific heat for various system sizes at 10^4 MC Sweeps (Solid lines) and 10^6 MC Sweeps (dotted lines). The figure showed a peak around $T \approx 0.5$ which indicated the Neel temperature.

The sharp peak in the main plot in **Figure 9** corresponds to the emergence of magnetic order in the system, we examine higher temperatures in this figure to show more accurate calculation of Neel temperature and what would be the behavior of the system at higher temperatures. The thermal excitations rapidly disrupt the ordered state as T increases.

The inset provides a detailed view of the specific heat around the peak, showing a series of smaller peaks. These features indicate complex internal phase transitions between magnetic states in the system. The decay and flattening of C at higher temperature state where specific heat becomes almost temperature-independent.

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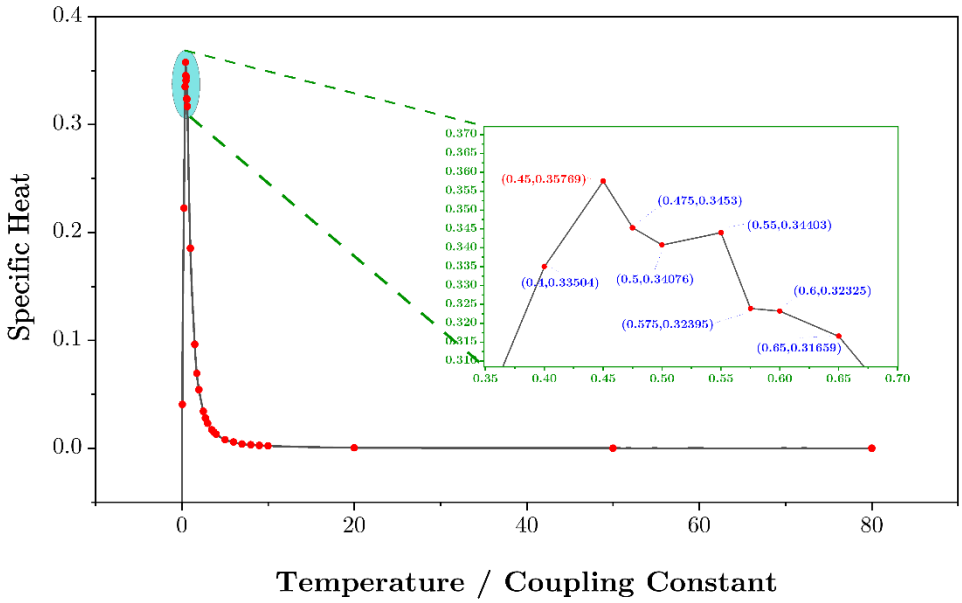

Figure 9: Specific heat over a wide range of temperatures where the inset figure focuses on the peak region. The results drop rapidly from a high value at $T \approx 0$ and gradually flattening out at higher temperatures. The inset zooms on the peak, highlighting multiple local maxima and corresponding specific heat values.

CONCLUSIONS

The SSE method effectively simulates the ground state energy and sublattice magnetization but struggles with specific heat calculations at low temperatures, often yielding non-physical results. Insufficient bins lead to large fluctuations, and achieving convergence requires significantly more Monte Carlo sweeps, increasing computational cost. The study identifies phase transitions and sharper peaks in specific heat for larger systems.

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Conflict of interests.

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الخلاصة

المقدمة:

النظم الانتيفيرومغناطيسية تُبدي سلوكاً معقداً يتطلب طرقاً رقمية دقيقة لتحليله. توسيع المتسلسلة العشوائي (SSE) هي طريقة من طرق مونتي كارلو الكمية التي تُستعمل لمحاكاة هذه الأنظمة. تختبر هذه الدراسة تأثير عدد التجميعات على دقة القياسات للخواص المغناطيسية باستعمال طريقة SSE.

طرق العمل:

تم اجراء محاكاة SSE باستعمال لغة Fortan 90 على معالج Ryzen 7. وقد تمت تهيئة النظام في درجات حرارة بدون ابعاد (32/1، 16/1، 2/1، و 4) وحجوم شبيكية (64، 128، 256، و 1024) مختلفة لفحص الترتيبات المختلفة له. وقد تم تغيير عدد التجميعات وعدد خطوات مونتي كارلو بطريقة منهجية لدراسة تاثيرهما على النتائج. تم رسم النتائج باستخدام برنامج Origin Lab.

النتائج:

ان زيادة عدد التجميعات (عدد الصناديق) يقلل من التقلبات، ويؤدي الى نتائج يمكن اعتمادها خصوصاً في درجات الحرارة الواطئة. ان درجات الحرارة الواطئة ادت الى وجود تقلبات اكبر في الحرارة النوعية والتاثرية المغناطيسية للنظام.

وقد تم رصد درجة حرارة نيل عند درجة حرارة نسبية تساوي تقريبا 0.5 (خالية من الوحدات) مشيرة الى حدوث انتقال طوري في هذه النقطة.

الاستنتاجات:

أظهرت هذه الدراسة أهمية عدد التجميعات على دقة النتائج في محاكاة اتساع المتسلسلة العشوائي. وعلى الرغم من كون التقنية فعالة لاغلب الخواص، لكن حسابات الحرارة النوعية تتطلب كلفة حسابية اعلى وتظهر محدودية في الدقة.

الكلمات المفتاحية: الشبيكة الخطية، توسيع المتسلسلة العشوائي، برم-2/1، انتيفيرومغناطيس، مونتي كارلو الكمية.

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