行政院國家科學委員會補助專題研究計畫 ■成果報告 □期中進度報告

低維量子自旋系統之研究

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計畫主持人：楊明峰
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行政院國家科學委員會專題研究計畫成果報告

低維量子自旋系統之研究

Study on low-dimensional quantum spin systems

計畫編號：NSC 96-2112-M-029 -004 -MY3
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一、中文摘要

最近，向濤與翁征宇等人，在將張量乘積態作為基態波函數的近似的基礎上，結合張量的重正化群計算，提出了一套通過投影方法來精確計算基態波函數的新方法 [H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 101, 090603 (2008)]。這個方法一方面大幅提高了可計算的張量維數和計算精確度，另一方面它可以輕易的處理大尺寸系統，因而避免有限尺寸效應所造成的影響。

在本計畫中，我們利用上述的方法來研究自旋 1/2 的反鐵磁 XXZ 模型在正方晶格上的磁化行為。在大的自旋異向性的情況下，我們的確觀察到，在磁化過程中，系統會出現一個一階的自旋翻轉相變。我們計算得出的相變點的數值以及各種物理量在相變點前後的差值均和目前最好的量子蒙特卡羅計算的結果可比擬。這顯示出，結合張量乘積態與張量重正化群的計算方法亦適用於來探討二維的一階量子相變問題。

關鍵詞：XXZ 模型，張量乘積態，量子相變

Abstract

By means of the recently proposed algorithm based on the tensor product states [H. C. Jiang, Z. Y. Weng, and T. Xiang, Phys. Rev. Lett. 101, 090603 (2008)], the magnetization process of the spin-1/2 anti-ferromagnetic XXZ model on a square lattice is investigated. In the large spin-anisotropy limit, clear evidence of a first-order spin-flip transition is observed as an external magnetic field is increased. Our findings of the critical field and the discrete jumps in various local order parameters are in good agreement with the quantum Monte Carlo data in the literature. Our results imply that this algorithm can be an accurate and efficient numerical approach in studying first-order quantum phase transitions in two dimensions.

Keywords: XXZ model, tensor product states, quantum phase transitions

二、緣由與目的、結果與討論

Numerical simulations are usually required in the theoretical investigation on strongly correlated systems, because analytical solutions are not available in most cases. Consequently, developing accurate and efficient numerical tools becomes one of the central issues in the understanding of quantum many-body systems. Recently, based on an efficient representation of two-dimensional system’s wave function through a tensor network, a series of new simulation algorithms has been achieved. In particular, the infinite projected entangled-pair states (iPEPS) algorithm [1] has been proposed and applied to various interesting systems with success [2–6]. In this approach, the ground-state wave function is described by the so-called tensor product state (TPS) [7,8] or the projected entangled-pair state (PEPS) [9,10]. Taking into account possible translational symmetry in the ground state, such a tensor network can be simply represented by copies of a small number of tensors even for systems on infinite lattices. After optimizing these tensors under specific prescriptions, a number of physical properties can be calculated from the optimized TPS/PEPS.

By handling tensor-product wave functions in different manners, schemes distinct from iPEPS algorithm have also been put forward [11,12]. A virtue of these approaches is that they can be implemented with ease. In Ref. [11], the optimized TPSs are determined via direct variational approach, where the variational energies of systems of very large sizes are efficiently evaluated by means of the tensor renormalization group (TRG) method [13,14]. The expectation values of physical quantities are then calculated from the optimized TPS again under the TRG method. This algorithm has been tested for several two-dimensional (2D) quantum spin models [11], and the results agree well with previous findings. Alternatively in Ref. [12], the ground states of a TPS form are obtained by using the power method through iterative projections. This approach can be considered as a generalization of the 1D infinite time-evolving block decimation (iTEBD) method [15] to the two dimensional cases. After getting the ground states, the TRG method [13] is employed to calculate the expectation values of physical observables. It is shown that accurate results for the Heisenberg model on a honeycomb lattice can be reached under this approach [12].

Due to the simplicity and efficiency of the iTEBD and the TRG algorithms, the approach proposed in Ref. [12] can become one of the promising numerical methods in studying quantum many-body systems once its general validity is established. Recently, it is shown that TPS/PEPS ansatz is suited to study the first-order phase transition [3]. However, because of the difference in optimizing ground states and in evaluating expectation values, one may wonder if the combined iTEBD and TRG algorithm can determine the first-order phase transitions to the same accuracy as the iPEPS algorithm does.

In order to provide further benchmark on the performance of the combined iTEBD and TRG algorithm, in this work [16] we investigate the magnetization process of the spin-1/2 anti-ferromagnetic XXZ model on a square lattice. Here the large spin-anisotropy case is considered, where the existence of first-order spin-flip transitions in the magnetization process has been established by means of quantum Monte Carlo (QMC) simulations. We find that various local order parameters defined below change discontinuously at a critical field, which clearly indicates the appearance of a first-order transition. Moreover, satisfactory results of the critical field and the discrete jumps in the local order parameters are be obtained as compared to the previous QMC findings. Our present investigation suggests that this combined algorithm should also be an effective numerical method in studying first-order quantum phase transitions in two dimensions.

三、計畫成果自評

由上述的結果可以看出，我們的工作提供了張量重整化群方法在量子自旋模型的應用的一個新例證。這對於國內外相關的後續研究工作有著相當程度的幫助。

由於這個結合張量乘積態與張量重正化群的計算方法沒有負概率問題，所以比量子蒙特卡羅方法可應用的範圍要廣得多。而且利用系統的對稱性質，還可進一步把精度提高好幾個數量級。因此這個新的數值計算方法未來將為強關聯物理的研究提供一個強有力的工具，來解決和澄清許多二維量子系統中的物理問題。

此外，相關的研究成果[17]均已刊登至 Physical Review B。

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