TNSPackage: A Fortran2003 library designed for tensor network state methods

Shao-Jun Dong, Wen-Yuan Liu, Chao Wang, Yongjian Han, G-C Guo, Lixin He

PII: S0010-4655(18)30078-X
DOI: https://doi.org/10.1016/j.cpc.2018.03.006
Reference: COMPHY 6451

To appear in: Computer Physics Communications

Received date: 13 June 2017
Revised date: 27 February 2018
Accepted date: 3 March 2018

Please cite this article as: S.-J. Dong, W.-Y. Liu, C. Wang, Y. Han, G.-C. Guo, L. He, TNSPackage: A Fortran2003 library designed for tensor network state methods, Computer Physics Communications (2018), https://doi.org/10.1016/j.cpc.2018.03.006

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.
TNSPackage: A Fortran2003 library designed for tensor network state methods

Shao-Jun Dong\textsuperscript{a,b}, Wen-Yuan Liu\textsuperscript{a,b}, Chao Wang\textsuperscript{a,b}, Yongjian Han\textsuperscript{a,b,*}, G-C Guo\textsuperscript{a,b}, Lixin He\textsuperscript{a,b,*}

\textsuperscript{a}CAS Key Laboratory of Quantum Information, University of Science and Technology of China, Hefei, Anhui, 230026, China
\textsuperscript{b}Synergetic Innovation Center of Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui, 230026, China

Abstract

Recently, the tensor network states (TNS) methods have proven to be very powerful tools to investigate the strongly correlated many-particle physics in one and two dimensions. The implementation of TNS methods depends heavily on the operations of tensors, including contraction, permutation, reshaping tensors, SVD and so on. Unfortunately, the most popular computer languages for scientific computation, such as Fortran and C/C++ do not have a standard library for such operations, and therefore make the coding of TNS very tedious. We develop a Fortran2003 package that includes all kinds of basic tensor operations designed for TNS. It is user-friendly and flexible for different forms of TNS, and therefore greatly simplifies the coding work for the TNS methods.

Keywords: Tensor Network State; Condensed Matter Physics;

PROGRAM SUMMARY

Program Title: TNSP
Program Files doi: http://dx.doi.org/10.17632/fggdbrndnx.1
Licensing provisions: GNU General Public License version 3
Programming language: Fortran2003
External routines: BLAS, LAPACK, ARPACK
Nature of problem: The implementation of Tensor Network State (TNS) methods depends heavily on the operations of tensors. Unfortunately, the most popular computer languages for scientific computation, such as Fortran and C/C++ do not have a standard library for such operations, and therefore make the coding of TNS very tedious.
Solution method: We develop a Fortran2003 package that includes all kinds of basic tensor operations designed for TNS, which greatly simplifies the coding work for the TNS methods.
Additional comments including Restrictions and Unusual features: A gcc-4.8.4 or later version is required to compile the code.

1. Introduction

One of the biggest challenges in modern condensed matter physics is to develop efficient numerical methods to solve the strongly correlated many-particle physics. As for strongly interacting systems, where conventional perturbation theory fails, numerical simulation plays a crucial role to reveal the nature of quantum many-body physics. Several popular methods, including the exact diagonalization (ED), Quantum Monte Carlo (QMC) methods [1, 2] and the density matrix renormalization group (DMRG) method [3, 4], have been widely used and achieve great success. However, there are some limitations for the previous methods: ED methods suffer from the “Exponential Wall” problem and the QMC suffers the notorious sign problem when simulating frustrated systems and fermion systems [5], whereas DMRG is limited to 1D or quasi-1D systems and does not work well for higher dimension systems [6]. It is pressing to develop new efficient numerical algorithms.

Recently, tensor network states (TNS), including matrix product states (MPS) [7], projected entangled pair states (PEPS) [8] etc., are proposed to describe many-body physics inspired by the quantum entanglement theory. The TNS
دریافت فوری
متن کامل مقاله

امکان دانلود نسخه تمام متن مقالات انگلیسی
امکان دانلود نسخه ترجمه شده مقالات
پذیرش سفارش ترجمه تخصصی
امکان جستجو در آرشیو جامعی از صدها موضوع و هزاران مقاله
امکان دانلود رایگان ۲ صفحه اول هر مقاله
امکان پرداخت اینترنتی با کلیه کارت های عضو شتاب
دانلود فوری مقاله پس از پرداخت آنلاین
پشتیبانی کامل خرید با بهره مندی از سیستم هوشمند رهگیری سفارشات