Quantum Control

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by

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Certificate

*This is to certify that the work contained in this thesis entitled **“Quantum Control"** is a bonafide work of **Hristo Tonchev** (60289), carried out in the Theoretical Physics Department, Sofia University under my supervision and that it has not been submitted elsewhere for a degree.*

Sofia
November 10, 2021

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Abstract

Tensor product state (TPS) based methods are powerful tools to efficiently simulate quantum many-body systems in and out of equilibrium. In particular, the one-dimensional matrix-product (MPS) formalism is by now an established tool in condensed matter theory and quantum chemistry. In these lecture notes, we combine a compact review of basic TPS concepts with the introduction of a versatile tensor library for Python (TeNPy) [1]. As concrete examples, we consider the MPS based time-evolving block decimation and the density matrix renormalization group algorithm. Moreover, we provide a practical guide on how to implement abelian symmetries (e.g., a particle number conservation) to accelerate tensor operations.

Chapter 1

Introduction

The interplay of quantum fluctuations and correlations in quantum many-body systems can lead to exciting phenomena. Celebrated examples are the fractional quantum Hall effect [2, 3], the Haldane phase in quantum spin chains [4, 5], quantum spin liquids [6], and hightemperature superconductivity [7]. Understanding the emergent properties of such challenging quantum many-body systems is a problem of central importance in theoretical physics. The main difficulty in investigating quantum many-body problems lies in the fact that the Hilbert space spanned by the possible microstates grows exponentially with the system size. To unravel the physics of microscopic model systems and to study the robustness of novel quantum phases of matter, large scale numerical simulations are essential. In certain systems where the infamous sign problem can be cured, efficient quantum Monte Carlo (QMC) methods can be applied. In a large class of quantum many-body systems (most notably, ones that involve fermionic degrees of freedom or geometric frustration), however, these QMC sampling techniques cannot be used effectively. In this case, tensor-product state based methods have been shown to be a powerful tool to efficiently simulate quantum many-body systems. The most prominent algorithm in this context is the density matrix renormalization group (DMRG) method [8] which was originally conceived as an algorithm to study ground state properties of one-dimensional (1D) systems. The success of the DMRG method was later found to be based on the fact that quantum ground states of interest are often only slightly entangled (area law), and thus can be represented efficiently using matrix-product states (MPS) [9–11]. More recently it has been demonstrated that the DMRG method is also a useful tool to study the physics of two-dimensional (2D) systems using geometries such as a cylinder of finite circumference so that the quasi-2D problem can be mapped to a 1D one [12]. The DMRG algorithm has been successively improved and made more efficient. For example, the inclusion of Abelian and non-Abelian symmetries, [13–17], the introduction of single-site optimization with density matrix perturbation [18, 19], hybrid real-momentum space representation [20, 21], and the development of real-space parallelization [22] have increased the convergence speed and decreased the requirements of computational resources. An infinite version of the algorithm [23] has facilitated the investigation of translationally invariant systems. The success of DMRG was extended to also simulate real-time evolution allowing to study transport and non-equilibrium phenomena, [24–29]. However, the bipartite entanglement of pure states generically grows linearly with time, leading to a rapid exponential growth of the computational cost. This limits time evolution to rather short times. An exciting recent development is the generalization of DMRG to obtain highly excited states of many-body localized systems [30–32] (see also [33] for a different approach). Tensor-product states (TPS) or equivalently projected entangled pair states (PEPS), are a generalization of MPS to higher dimensions [34,35]. This class of states is believed to efficiently describe a wide range of ground states of two-dimensional local Hamiltonians. TPS serve as variational wave functions that can approximate ground states of model Hamiltonians. For this several algorithms have been proposed, including the Corner Transfer Matrix Renormalization Group Method [36], Tensor Renormalization Group (TRG) [37], Tensor Network Renormalization (TNR) [38], and loop optimizations [39].

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Chapter 3

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