



Abschlussarbeit im Masterstudiengang Physik der  
Kondensierten Materie

# **Entwicklung eines diagonalen isometrischen Tensor Netzwerk Algorithmus**

**Development of a diagonal isometric Tensor Network Algorithm**

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I hereby declare that this thesis is entirely the result of my own work except where otherwise indicated. I have only used the resources given in the list of references.

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## Abstract

The numerical simulation of strongly interacting quantum many-body systems is a challenging problem. In the last decades, Tensor Networks have emerged as the standard method for tackling this problem in one dimensional systems in the form of Matrix Product States (MPS). Tensor Networks have also been generalized for the highly relevant problem of two and more spatial dimensions. However, these so-called Projected Entangled Pair States (PEPS) are typically plagued by high computational complexity or drastic approximations. Recently, a new class of Tensor Networks, called isometric Tensor Networks, have been proposed for the simulation of two-dimensional quantum systems. This new class of Tensor Networks can be understood as a generalization of the one-dimensional Matrix Product States to higher dimensions. While isometric Tensor Networks generally capture only a subspace of the total Hilbert space, there are already promising results. In this work, we develop a new class of isometric Tensor Networks that has some key differences to the existing one. We show first numerical results for finding ground states of the Transverse Field Ising model.

## Zusammenfassung



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# **Chapter 1**

## **Introduction**





# Chapter 2

## Tensors and Tensor Networks

### 2.1 Tensors and Isometries

For the purpose of this thesis a *tensor*  $T$  of rank  $n$  is an  $n$ -dimensional array of complex numbers

$$T \in \mathbb{C}^{\chi_1 \times \chi_2 \times \dots \times \chi_n}, \quad \chi_i \in \{1, 2, \dots\}$$

with entries

$$T_{i_1 i_2 \dots i_n} \in \mathbb{C}, \quad i_j \in \{1, 2, \dots, \chi_j\}.$$

With this definition, a rank-0 tensor is a scalar, a rank-1 tensor is a vector, and a rank-2 tensor is a matrix. It is convenient to introduce a diagrammatic notation, where tensors are drawn as shapes and tensor indices are drawn as lines (*legs*) emerging from the shapes. To relate this diagrammatic notation to equations, one often decorates each line with the corresponding index  $i_j$ . A scalar, vector, matrix, and a general rank- $n$  tensor are visualized in this notation in figure 2.1.

A *tensor contraction* between two tensors along one or multiple indices is the linear operation that is given by summing over all contracted indices. Given a rank- $(n + f)$

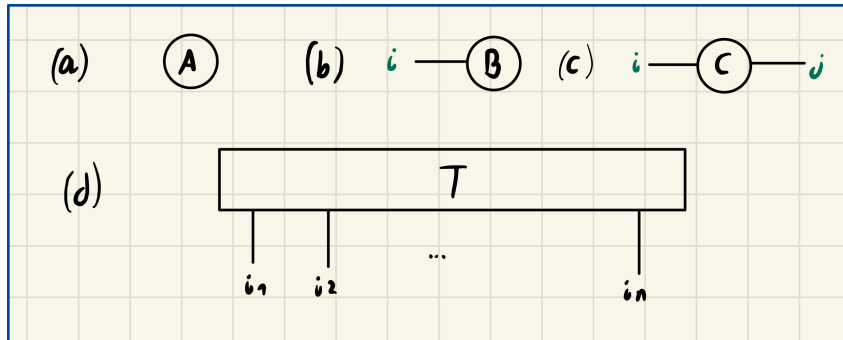


Figure 2.1: Tensors of different ranks are shown in diagrammatic notation. (a) A scalar  $a \in \mathbb{C}$ . (b) A vector  $\mathbf{b} \in \mathbb{C}^\chi$ . (c) A matrix  $\mathbf{C} \in \mathbb{C}^{\chi_1 \times \chi_2}$ . (d) A rank- $n$  tensor  $T \in \mathbb{C}^{\chi_1 \times \chi_2 \times \dots \times \chi_n}$

tensor  $\mathbf{X} \in \mathbb{C}^{\chi_1 \times \dots \times \chi_n \times \xi_1 \times \dots \times \xi_f}$  and a rank- $(m + f)$  tensor  $\mathbf{Y} \in \mathbb{C}^{\lambda_1 \times \dots \times \lambda_m \times \xi_1 \times \dots \times \xi_f}$ , the result of contracting  $\mathbf{X}$  and  $\mathbf{Y}$  along the last  $f$  indices produces a new rank- $(m + n)$  tensor  $\mathbf{Z} \in \mathbb{C}^{\chi_1 \times \dots \times \chi_n \times \lambda_1 \times \dots \times \lambda_m}$  as

$$Z_{i_1 \dots i_n j_1 \dots j_m} := \sum_{\alpha_1=1}^{\xi_1} \dots \sum_{\alpha_f=1}^{\xi_f} X_{i_1 \dots i_n \alpha_1 \dots \alpha_f} Y_{j_1 \dots j_m \alpha_1 \dots \alpha_f}.$$

Arbitrary contractions can be reformulated as contractions over the last  $f$  indices by transposing the tensors. By counting the number of multiplications and additions that are necessary to perform the contraction, the computational complexity can be determined as

$$\mathcal{O} \left( \prod_{\mu=1}^n \chi_{\mu} \prod_{\mu=1}^m \lambda_{\mu} \prod_{\mu=1}^f \xi_{\mu} \right).$$

A *tensor network* is defined as a collection of tensors that are contracted in a given way. For example, the matrix-vector product of the matrix  $\mathbf{A} \in \mathbb{C}^{\chi_1 \times \chi_2}$  and the vector  $\mathbf{b} \in \mathbb{C}^{\chi_2}$  can be written as the contraction of a rank-2 tensor with a rank-1 tensor, resulting in a rank-1 tensor  $\mathbf{b}' \in \mathbb{C}^{\chi_1}$  with entries

$$b'_i = \sum_{\alpha=1}^{\chi_2} A_{i\alpha} b_{\alpha}. \quad (2.1)$$

The matrix product of two matrices  $\mathbf{A} \in \mathbb{C}^{\chi_1 \times \chi_2}$  and  $\mathbf{B} \in \mathbb{C}^{\chi_2 \times \chi_3}$  can be written as a tensor network of two rank-2 tensors,

$$C_{ij} = \sum_{\alpha=1}^{\chi_2} A_{i\alpha} B_{\alpha j}, \quad (2.2)$$

where the result is another rank-2 tensor  $\mathbf{C} \in \mathbb{C}^{\chi_1 \times \chi_3}$ . As a more involved example we look at a tensor network consisting of two rank-3 tensors  $\mathbf{A} \in \mathbb{C}^{\chi_1 \times \chi_2 \times \chi_3}$  and  $\mathbf{B} \in \mathbb{C}^{\chi_2 \times \chi_4 \times \chi_5}$  and one rank-4 tensor  $\mathbf{C} \in \mathbb{C}^{\chi_3 \times \chi_5 \times \chi_6 \times \chi_7}$ , where we contract along the dimensions  $\chi_2$ ,  $\chi_3$  and  $\chi_5$ . The result is a rank-4 tensor  $\mathbf{D} \in \mathbb{C}^{\chi_1 \times \chi_4 \times \chi_6 \times \chi_7}$ :

$$D_{ijkl} = \sum_{\alpha=1}^{\chi_2} \sum_{\beta=1}^{\chi_3} \sum_{\gamma=1}^{\chi_5} A_{i\alpha\beta} B_{\alpha j\gamma} C_{\beta\gamma kl}. \quad (2.3)$$

In tensor network diagrams, contractions are visualized by connecting the lines corresponding to contracted indices. In figure 2.2 we show tensor network diagrams for the tensor networks (2.1), (2.2) and (2.3).

Because tensor contractions are linear, the order in which tensors are contracted doesn't change the result. However, the computational complexity does in general depend on the order of contractions and can thus be minimized by choosing the optimal contraction order.

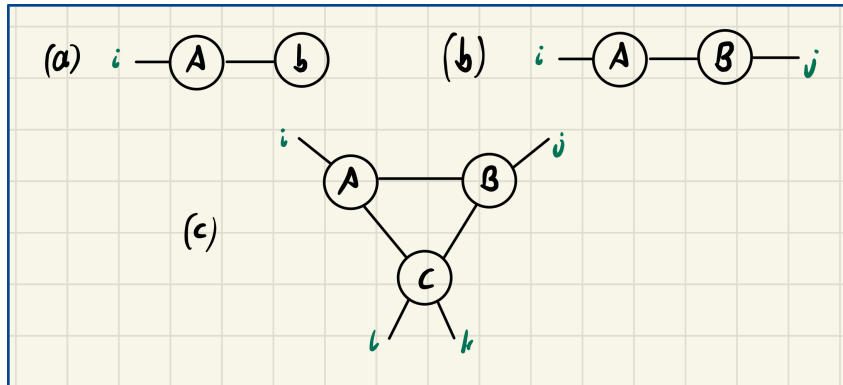


Figure 2.2: Different simple tensor networks are shown in diagrammatic notation. (a) matrix-vector product (2.1). (b) matrix-matrix product (2.2). (c) Tensor network consisting of three tensors (2.3).

## 2.2 Matrix Product States (MPS)

## 2.3 isometric Tensor Networks in 2D



## **Chapter 3**

# **Isometric Diagonal Tensor Networks (isoDTPS)**

### **3.1 Network Structure**

### **3.2 Yang-Baxter Move**

### **3.3 Time Evolving Block Decimation (TEBD)**



## **Chapter 4**

### **Toric Code: An exactly representable Model**





## **Chapter 5**

### **Transverse Field Ising Model: Ground State Search and Time Evolution**



# Appendix A

## Riemannian Optimization of Isometries

In this appendix we provide a brief introduction to the problem of optimizing a cost function on the constrained set of isometric matrices. This problem can be solved by performing Riemannian Optimization on the matrix manifold of isometric matrices, which is called the Stiefel manifold. For a more in-depth introduction to the topic we recommend the excellent book [1]. A discussion of Riemannian optimization of complex matrix manifolds in the context of quantum physics and isometric tensor networks can be found at [2, 3]. An implementation of Riemannian Optimization on the real Stiefel manifold and other matrix manifolds in python is given in [4]. Some parts of this implementation were also used in our implementation.

### A.1 The complex Stiefel manifold

We define the *complex Stiefel manifold*  $\text{St}(n, p)$  with  $n \geq p$  as the set of all isometric  $n \times p$  matrices:

$$\text{St}(n, p) := \left\{ X \in \mathbb{C}^{n \times p} : X^\dagger X = \mathbb{1} \right\}.$$

In particular, for  $n = p$ , the complex Stiefel manifold reduces to the set of unitary matrices  $U(n)$ . One can show, similar to [1], that the complex Stiefel manifold is naturally an embedded submanifold of the Euclidian vector space  $\mathbb{C}^{n \times p} \cong \mathbb{R}^{2np}$  of general complex  $n \times p$  matrices.

Tangent vectors on manifolds generalize the notion of directional derivatives. A mathematical definition of tangent vectors and tangent spaces of manifolds is given in [1]. The set of all tangent vectors to a point  $X \in \text{St}(n, p)$  is called the *tangent space*  $T_X \text{St}(n, p)$ , which is given by [1, 3]

$$T_X \text{St}(n, p) = \left\{ Z \in \mathbb{C}^{n \times p} : X^\dagger Z + Z^\dagger X = 0 \right\}.$$

An arbitrary element  $\xi \in \mathbb{C}^{n \times p}$  from the embedding space  $\mathbb{C}^{n \times p}$  can be projected to the tangent space  $T_X \text{St}(n, p)$  by [1, 3]

$$P_X \xi = \xi - \frac{1}{2} X \left( X^\dagger \xi + \xi^\dagger X \right). \quad (\text{A.1})$$

Additionally, we will also need to define a notion of length that we can apply to tangent vectors. This can be done in the form of an *inner product* on tangent spaces, called the *Riemannian metric*. A natural metric for the tangent space  $T_X \text{St}(n, p)$  of the Stiefel manifold is the Euclidean metric of the embedding space  $\mathbb{C}^{n \times p}$ , which is given by the real part of the Frobenius inner product:

$$g_W : T_X \text{St}(n, p) \times T_X \text{St}(n, p) \rightarrow \mathbb{R}, \quad g_X(\xi_1, \xi_2) = \text{Re Tr} \left( \xi_1^\dagger \xi_2 \right). \quad (\text{A.2})$$

Equipped with a Riemannian metric the Stiefel manifold becomes a Riemannian submanifold of  $\mathbb{C}^{n \times p}$ .

With these definition, we can now formulate the optimization problem as the problem of finding the isometry  $W_{\text{opt}} \in \text{St}(n, p)$  that minimizes the cost function

$$f : \text{St}(n, p) \rightarrow \mathbb{R}, \quad X \mapsto f(X). \quad (\text{A.3})$$

## A.2 Gradients, retractions, and vector transport

First order optimization algorithms like Gradient Descent and Conjugate Gradients use the gradient of the cost function to update the search direction at each iteration. In the case of the Stiefel manifold and the cost function (A.3), we first define the matrix of partial derivatives  $D \in \mathbb{C}^{n \times p}$  of  $f$  at  $X \in \text{St}(n, p)$  by

$$D_{ij} := \left. \frac{\partial f}{\partial \text{Re}(X_{ij})} \right|_X + i \left. \frac{\partial f}{\partial \text{Im}(X_{ij})} \right|_X. \quad (\text{A.4})$$

With this definition, the directional derivative  $Df(X)[Z]$  at  $X \in \text{St}(n, p)$  in direction  $Z \in \mathbb{C}^{n \times p}$  is simply given by an inner product of  $D$  with the direction  $Z$ , using the Riemannian metric (A.2):

$$\begin{aligned} g_X(D, Z) &= \text{Re Tr} \left( D^\dagger Z \right) = \text{Re} \sum_{ij} D_{ij}^* Z_{ij} \\ &= \sum_{ij} \left( \left. \frac{\partial f}{\partial \text{Re}(X_{ij})} \right|_X \text{Re } Z_{ij} + \left. \frac{\partial f}{\partial \text{Im}(X_{ij})} \right|_X \text{Im } Z_{ij} \right) \\ &=: Df(X)[Z]. \end{aligned}$$

With this we can now define the gradient  $\nabla f(X)$  of  $f$  at  $X \in \text{St}(n, p)$  as the projection of the partial derivative matrix (A.4) to the tangent space [1, 3]:

$$\nabla f(X) := P_X D = D - \frac{1}{2} X \left( X^\dagger D + D^\dagger X \right),$$

where we used the projection (A.1).

### **A.3 Conjugate Gradients**

### **A.4 Trust Region Method**



## **Appendix B**

### **Initialization of the Disentangling Unitary**





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