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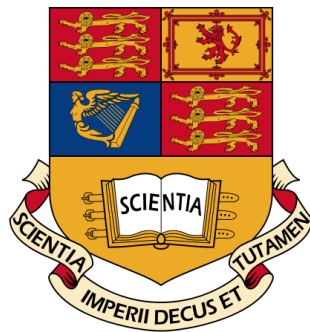
Continuous Matrix Product State Representations for Quantum Field Theory

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Abstract

In this MSc dissertation we investigate the recently introduced continuous matrix product state formalism (cMPS), which lies at the intersection between quantum information theory and quantum field theory. Quantum information theoretic concepts allow for an efficient description of quantum field states with the states obeying an area law. This efficiency in description of what has been christened the physical corner of Hilbert space allows us to apply the variational method to quantum fields, a goal that has been a long-standing challenge for field theorists. In this thesis, we will derive core aspects of this formalism and apply it to the non-relativistic Lieb-Liniger model and the relativistic free Dirac model, carefully going through our numerical implementations and results and illustrating technical and physical subtleties involved in the machinery of the cMPS formalism when used as a variational method. We present a new technique for demonstrating an aspect of Dirac theory, where we solve dissipative dynamics on an auxiliary system to show the filling of the Dirac sea. We conclude with an outlook onto future roads of research.

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Contents

Abstract	i
1 Introduction	1
1.1 From entanglement to matrix product states	1
1.2 Outline of this dissertation	3
2 The Variational Principle	4
2.1 The Rayleigh-Ritz method	4
2.2 Desiderata for a variational class	6
2.3 Entropic area laws for local Hamiltonians	6
3 Matrix Product State Representations	8
3.1 Singular value decomposition	9
3.2 Schmidt decomposition	9
3.3 Matrix Product Representation	11
3.4 Normal form	12
3.5 Boundary conditions	13
3.6 Gauge freedom	13
3.7 MPS and entanglement	14

3.8	Expectation values	14
4	Continuous Matrix Product States	16
4.1	Generic state	16
4.2	Expansion in the field operators	17
4.3	Derivation of cMPS as continuum limit of MPS	18
4.4	cMPS from continuous measurement	19
4.5	Expectation values in cMPS	21
4.6	Gauge freedom for cMPS	24
4.7	Translation invariance	25
4.8	The cMPS dictionary for expectation values	25
4.9	Useful isomorphisms	26
4.10	Lindblad equation	27
4.11	Thermodynamic limit	29
4.12	Steady state for expectation values	30
5	The Lieb-Liniger model	32
5.1	Lieb-Liniger Hamiltonian	33
5.2	Ground state	33
5.3	Tonks-Girardeau limit	34
5.4	Number operator	34
5.5	Minimization	35
6	Free Dirac model	37
6.1	Dirac equation	38
6.2	Lagrangian and Hamiltonian	38

6.3	cMPS for multiple particle species	39
6.4	Picking up a minus sign	40
6.5	Jordan-Wigner transformation	42
6.6	Expectation values	44
6.7	Solution of the quantized Dirac equation	44
6.8	Momentum space occupation-number	47
6.9	Large momentum behaviour	49
6.10	Scale transformations	50
6.11	Regularisation	51
6.12	Description of our algorithm	52
6.13	Dirac sea	53
7	Conclusion and Outlook	57
7.1	Conclusion	57
7.2	Outlook	58
8	Appendix	60
8.1	Lieb-Liniger code	60
8.2	Dirac code	64
	Bibliography	71

Conventions and preliminaries

Before diving into the matter, let us establish our conventions and provide some key results and properties, which we make repeated use of.

- \mathcal{T} and \mathcal{P} denote time-ordering and path-ordering respectively
- Einstein summation, i.e. implicit summing over indices that appear twice in a product, with one upstairs and one downstairs
- $*$ denotes complex and \dagger Hermitian conjugation
- σ^i denote the Pauli matrices

$$\sigma^1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- density matrix $\rho \in \mathcal{L}(\mathcal{H})$ for $|\psi\rangle \in \mathcal{H}$

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \quad \text{tr } \rho = 1 \quad \rho \geq 0$$

- partial trace: for a composite system $\rho_{AB} \in \mathcal{L}(\mathcal{H}_A \otimes \mathcal{H}_B)$

$$\rho_A = \text{tr}_B \{ \rho_{AB} \} = \sum_k (\mathbb{1} \otimes \langle k|) \rho_{AB} (\mathbb{1} \otimes |k\rangle)$$

- Entanglement entropy: for a pure bipartite system $\rho_{AB} = |\psi\rangle_{AB} \langle \psi|$ the von-Neumann entropy is a unique measure of entanglement:

$$S(\rho_A) = -\text{tr}(\rho_A \log \rho_A)$$

- Clifford algebra in $1 + 1$ dimensions with $\eta_{\mu\nu} = \text{diag}(1, -1)$ and choice of γ_μ

$$\{\gamma_\mu, \gamma_\nu\} = 2\eta_{\mu\nu}\mathbf{1} \Leftrightarrow \gamma_0 = \sigma_z \quad \gamma_1 = i\sigma_x$$

- Commutator product rule:

$$[A, BC] = B[A, C] + [A, B]C$$

- Trace over tensor products:

$$\text{tr}(A \otimes B) = \sum_{ij} \langle ij | A \otimes B | ij \rangle = \sum_i \langle i | A | i \rangle \sum_j \langle j | B | j \rangle = \text{tr } A \text{tr } B$$

Credit

This thesis is based on the seminal work by Frank Verstraete, Ignacio Cirac, Tobias Osborne, Jutho Haegeman, Jens Eisert et al. [[Verstraete and Cirac, 2010](#), [Haegeman et al., 2010](#), [Haegeman, 2011](#)].

Chapter 1

Introduction

1.1 From entanglement to matrix product states

One of the most striking and astonishing features of quantum mechanics is the phenomenon of entanglement. Entanglement is a core concept in the theory of quantum information, where it lies at the heart of the theory's most famous results like the violation of Bell's theorem or quantum computing. Since then, the concept has spread into different areas of physics and there is hope that it might shed new light onto important questions. The first fundamental lesson quantum information theory teaches us is that Hilbert space is too big, which is to say physical states only populate a tiny part of Hilbert space. New and provably efficient representations of quantum field states can give us access to powerful new analytical tools to analyse quantum field systems, classify quantum phases and construct solvable non-trivial models. In addition, these representations naturally allow for variational methods for the calculation of physical properties of matter. The canonical example for

where this has happened is a method called the density matrix renormalization group (DMRG), which is a vastly successful method for the analysis of strongly correlated one-dimensional systems. The success of the DMRG method originates from the particular entanglement scaling in these systems, where the entanglement entropy obeys an area law. For example the entropy of a block of spins in one dimension scales like the boundary of the block and is therefore bounded by a constant. The method to incorporate this scaling of entropy is the matrix product state formalism. The matrix product state is a particular way to write a quantum state and forms part of a more general class of tensor network states. It allows to regulate the degree of entanglement in our description of a system. It has been observed that the ground states of most Hamiltonians obey such an area law [Eisert et al., 2010] and hence it is vastly inefficient to describe them by the naïve full Hilbert space description [Poulin et al., 2011]. This restriction to what we call the physical corner of Hilbert space, and which roughly speaking encodes the information from distant regions into the boundary, makes it possible to apply the variational principle to an otherwise intractable task, and thereby allows us to study quantum systems to new depths. In 2010, Verstraete and Cirac proposed a continuum limit of matrix product states, hence called the continuous matrix product state formalism [Verstraete and Cirac, 2010]. The motivation is again to use the variational principle but this time we subject our formalism not to lattice systems but to field theories, thereby making the connection to a wider range of physics. The area law scaling of the entanglement entropy, conjectured to be an instance of the general holographic principle, is a phenomenon that can also be found in the forementioned types

of theories. Looking back at the golden age of black holes one famous example is certainly the scaling of the entropy of black holes, which does scale like the area of the black hole and not as its volume and gave rise to black hole thermodynamics [Bekenstein, 1973]. History aside, the cMPS formalism is a promising direction of research for simulating field theories. The auxiliary fields we introduce in this formalism arise in a very similar manner in the context of cavity QED, which firstly will give us an intuitive interpretation for our method and secondly has recently been turned on its head and used to propose the simulation of quantum fields by using a cavity [Barrett et al., 2012].

1.2 Outline of this dissertation

In this dissertation, we will analyse the recently introduced cMPS formalism for efficiently handling quantum fields. We will demonstrate its effectiveness as a variational class by applying it to the Lieb-Liniger model, a model of a one dimensional bosonic gas. We go through the physical and numerical implementation details of the cMPS procedure. We then extend the formalism to a relativistic setting, where we use the free Dirac equation as a toy theory. The relativistic nature of this provides a good setting for illustrating various subtle features of the cMPS formalism and its ability to extract meaningful physics. The original work of this dissertation will be a new approach to finding the filling of the Dirac sea by solving the dissipative dynamics on the auxiliary system.

Chapter 2

The Variational Principle

2.1 The Rayleigh-Ritz method

The version of the variational principle we intend to use in this thesis is due to [Ritz \[1909\]](#). It states that the energy expectation value of any state will always be greater or equal to the energy of the ground state:

$$E^0 \leq \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \quad (2.1)$$

The proof is straightforward, if we use a completeness relation in the eigenbasis of the Hamiltonian [[Shankar, 1994](#)],

$$\mathbb{1} = \sum_E |E\rangle \langle E| \quad \hat{H} |E\rangle = E |E\rangle, \quad (2.2)$$

which we insert into the above expression

$$\begin{aligned}
 \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} &= \sum_E \frac{\langle \psi | \hat{H} | E \rangle \langle E | \psi \rangle}{\langle \psi | \psi \rangle} \\
 &= \sum_E E |\langle E | \psi \rangle|^2 (\langle \psi | \psi \rangle)^{-1} \\
 &\geq E^0 \sum_E |\langle E | \psi \rangle|^2 (\langle \psi | \psi \rangle)^{-1} = E^0.
 \end{aligned} \tag{2.3}$$

For the inequality in the last line we used that E^0 is by definition the lowest energy of the Hamiltonian and for the very last step we used the completeness relation in reverse.

Thus, at least in theory, we have a method to find the ground state of an arbitrary Hamiltonian: We take all states in the Hilbert space and for every state compute the energy expectation value. We then search for the pair $(|\psi\rangle, E_\psi)$ with the lowest energy and the corresponding vector is a good candidate for the ground state of the Hamiltonian in question. Alas, this already indicates the crucial problem with this method, because we would have to search through every possible state in Hilbert space. For example, if we have a spin-chain with n sites, we would have to search through all possible states

$$\sum_{\sigma_1 \dots \sigma_n} c_{\sigma_1 \dots \sigma_n} |\sigma_1 \dots \sigma_n\rangle, \tag{2.4}$$

where the number of coefficients $c_{\sigma_1 \dots \sigma_n}$ scales like 2^n . This exponential scaling of the size of Hilbert space with the system thus makes the naïve use of the variational principle an intractable search for the needle in the haystack.

2.2 Desiderata for a variational class

We would like to find a parametrization for a manifold of physical states, that provides us with the three following features:

- *Efficiency*: a polynomial scaling in parameters as we increase the system size
- *Completeness*: we would like to be able to reach all states in the full Hilbert space
- *Naturalness*: the physics should be described by local observables and the entanglement entropy should obey an area law

We see that the full Hilbert space description fails on point one and three, it has exponential scaling in parameters and the entropy obeys a volume law rather than an area law. The standard approach to the variational method so far has been to use Gaussian states. However, they fail on point two as they do not capture all states. In contrast to that cMPS is a good candidate for a variational class that satisfies all these requirements.

2.3 Entropic area laws for local Hamiltonians

If one takes a random state out of the full Hilbert space of a system, that state will be locally featureless and maximally entangled with its surrounding. However, ground-states of local Hamiltonians are only slightly entangled and typically obey the above mentioned entanglement-entropy area-laws [Eisert

et al., 2010]. The region of Hilbert space, which contains these slightly entangled states is actually an exponentially small [Poulin et al., 2011] part of the full Hilbert space and has been christened the “physical corner of Hilbert space”. A central goal of the matrix product states program is exactly to capture this behaviour, thereby “foliating” Hilbert space. If this parametrization has a favourable scaling, we are back in the game for the variational principle, since now the proverbial search for the needle in the haystack can be turned into a polynomially scaling problem, therefore allowing an efficient use of the variational method.

Chapter 3

Matrix Product State Representations

The matrix product state representation defines a natural hierarchy for any Hilbert space of quantum states. That is to say, any pure quantum state can be recast as a matrix product state. Writing a state as an MPS essentially amounts to expressing the coefficients of the state as matrix products which then gives the state several powerful and desirable features. Looking at the state $|\psi\rangle$ in the spin-basis

$$|\psi\rangle = \sum_{\sigma_1 \dots \sigma_n} c_{\sigma_1 \dots \sigma_n} |\sigma_1 \dots \sigma_n\rangle, \quad (3.1)$$

we can view the complex coefficient $c_{\sigma_1 \dots \sigma_n}$ as a tensor, which we will decompose into matrices by repeated use of singular value decomposition.

3.1 Singular value decomposition

Every rectangular matrix M admits a decomposition of the following form, called the singular value decomposition (SVD)

$$M = UDV^\dagger \quad (3.2)$$

with $UU^\dagger = \mathbf{1}$, $V^\dagger V = \mathbf{1}$ and D diagonal. So in components:

$$M_{ij} = \sum_k U_{ik} D_{kk} V_{jk}^*. \quad (3.3)$$

3.2 Schmidt decomposition

The Schmidt decomposition is canonical representation of pure bipartite quantum states. Given a bipartite system with Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$, any quantum state $|\psi\rangle \in \mathcal{H}_{AB}$

$$|\psi\rangle = \sum_{mn} a_{mn} |m\rangle_A |n\rangle_B \quad (3.4)$$

can be decomposed by bringing the coefficients a_{mn} into their SVD form

$$|\psi\rangle = \sum_{imn} u_{mi} d_{ii} v_{ni}^* |m\rangle_A |n\rangle_B. \quad (3.5)$$

Now u and v , since they are unitary, just rotate the basis states. This can be seen as a new orthonormal basis, which we write as

$$\sum_m u_{mi} |m\rangle_A =: |i\rangle_A \in \mathcal{H}_A \quad \sum_n v_{ni}^* |n\rangle_B =: |i\rangle_B \in \mathcal{H}_B. \quad (3.6)$$

Thereby we get to the standard form of the Schmidt decomposition

$$|\psi\rangle = \sum_{k=1}^r \sqrt{\lambda_k} |k\rangle_A |k\rangle_B \quad (3.7)$$

with orthonormal bases $|k\rangle_A$ and $|k\rangle_B$ as well as $\sum_k \lambda_k = 1$. The sum runs over the number of singular values of the original coefficient matrix a_{mn} , which is related to entanglement and is called the Schmidt-rank r of the state $|\psi\rangle$. The Schmidt rank is an example of what we in general will call the bond dimension and which plays a key role in our later analysis when we deal with multipartite systems. For a given Schmidt rank we can find an upper bound on the entanglement entropy. The reduced density matrix is

$$\rho_A = \text{tr}_B |\Psi\rangle \langle \Psi| = \sum_{k=1}^r \lambda_k |k\rangle \langle k| \quad \text{with} \quad \sum_k \lambda_k = 1. \quad (3.8)$$

The upper bound is given by $\lambda_k = 1/r$, which gives

$$S(\rho_A) = - \sum_{k=1}^r \lambda_k \log \lambda_k \leq - \sum_{k=1}^r \frac{1}{r} \log(r^{-1}) = \log r. \quad (3.9)$$

3.3 Matrix Product Representation

Let us now use eqn. (3.7) to decompose a general pure state of n sites

$$|\psi\rangle = \sum_{\sigma_1 \dots \sigma_n} c_{\sigma_1 \dots \sigma_n} |\sigma_1 \dots \sigma_n\rangle. \quad (3.10)$$

We recursively Schmidt-decompose the coefficient $c_{\sigma_1 \dots \sigma_n}$ as

$$c_{\sigma_1 \dots \sigma_n} = \sum_{k_1}^{D_{k_1}} U_{\sigma_1 k_1} d_{k_1 k_1} (V^\dagger)_{k_1 (\sigma_2 \dots \sigma_n)} = \quad (3.11)$$

$$\sum_{k_1} U_{\sigma_1 k_1} c_{k_1 \sigma_2 \dots \sigma_n} = \sum_{k_1 k_2} U_{\sigma_1 k_1} U_{(k_1 \sigma_2) k_2} c_{(a_2 \sigma_3) (\sigma_4 \dots \sigma_n)} = \dots \quad (3.12)$$

$$= \sum_{k_1 \dots k_{n-1}} U_{\sigma_1 k_1} U_{(k_1 \sigma_2) k_2} \dots U_{(k_{n-2} \sigma_{n-1}) k_{n-1}} U_{\sigma_n k_{n-1}}, \quad (3.13)$$

where we absorbed the singular value matrix d_{kk} into V^\dagger in every step and the k_i run from 1 to the bond dimension D_{k_i} . We can understand the k_i as the matrix indices, which make this into a matrix product and σ_i as labels to the individual matrices. Thus defining

$$A_{ab}^{\sigma_i} := U_{(a \sigma_i) b}, \quad (3.14)$$

we can now write the coefficients as a product over matrices

$$c_{\sigma_1 \dots \sigma_n} = A^{\sigma_1} \dots A^{\sigma_n}, \quad (3.15)$$

where we suppress the matrix indices and hence have found the matrix product state representation

$$|\Psi\rangle = \sum_{\sigma_1 \dots \sigma_n} A^{\sigma_1} \dots A^{\sigma_n} |\sigma_1 \dots \sigma_n\rangle. \quad (3.16)$$

3.4 Normal form

Due to the unitarity in the SVD matrices we have

$$U^\dagger U = \mathbf{1} \Leftrightarrow \sum_{j, \sigma_m} U^\dagger_{i \sigma_m j} U_{j \sigma_m k} = \delta_{ik} \quad (3.17)$$

$$\Rightarrow \sum_{\sigma_m} A^{\sigma_m \dagger} A^{\sigma_m} = \mathbf{1}, \quad (3.18)$$

which is called the left normalization condition [Schollwoeck, 2010], since we started our decomposition of $c_{\sigma_1 \dots \sigma_n}$ from the left and in the next step we will show it directly leads to a normalized state. We could equally well have started on the right and go in the other direction, which would give us the right normalized form $\sum AA^\dagger = \mathbf{1}$. Let us now compute the norm of the state as

$$\begin{aligned} \langle \Psi | \Psi \rangle &= \sum_{\sigma_1 \dots \sigma_n} (A^{\sigma_n})^\dagger \dots (A^{\sigma_1})^\dagger A^{\sigma_1} \dots A^{\sigma_n} = \\ &= \sum_{\sigma_n} (A^{\sigma_n})^\dagger \dots \left\{ \sum_{\sigma_2} (A^{\sigma_2})^\dagger \left\{ \underbrace{\sum_{\sigma_1} (A^{\sigma_1})^\dagger A^{\sigma_1}}_{=1} \right\} A^{\sigma_2} \right\} \dots A^{\sigma_n} = 1. \end{aligned} \quad (3.19)$$

We see that due to the left normalization condition everything contracts nicely and our state is normalized.

3.5 Boundary conditions

The first and last matrices are actually a row and a column vector respectively, which is the so called open boundary case. We could also promote them to matrices and trace over the whole matrix product, which is called the periodic boundary case. We combine these by writing

$$|\psi\rangle = \sum_{\sigma_1 \dots \sigma_n} \text{tr} B A^{\sigma_1} \dots A^{\sigma_n} |\sigma_1 \dots \sigma_n\rangle, \quad (3.20)$$

where $B = \mathbb{1}$ for periodic boundary conditions and $B = |\omega_R\rangle \langle \omega_L|$ for open boundary conditions. We note that local observables away from the boundary should not be able to distinguish between the two.

3.6 Gauge freedom

From the above form it is immediately apparent, that we have an overcomplete parametrization, since we are free to gauge a matrix $A[n]$ at site n by the transformation

$$A[n] \rightarrow X[n-1]A[n](X[n])^{-1} \quad (3.21)$$

with some invertible matrices X . Taken as a variational manifold, these are gauge degrees of freedom, which leave the physical state unaffected.

3.7 MPS and entanglement

It is clear from the generality of the Schmidt decomposition, that if we let the bond dimension D go to infinity, we can capture any arbitrary state in the Hilbert space and thus our representation is complete. However, up to this point, one might wonder what the benefit might be, since we so far have added more to the state instead of reducing it. The key insight is, that the bond dimension, analogously to the Schmidt rank, is related to the amount of entanglement encoded in the state. One extreme is the above mentioned arbitrarily large bond dimension and the other extreme is a bond dimension of one, where we then are multiplying scalars and hence have a classical product state with no entanglement. The physical states lie between these extremes and with moderate bond dimension we can capture any physical state, at the same time avoiding the significant overhead which is present in the generic Hilbert space description (eqn. 3.10). For example, $D = 2$ or 3 is already sufficient to describe states as significant as W-states, GHZ-states and cluster-states. In complete analogy with eqn. (3.9) the upper bound on the entanglement entropy is again given by $S \leq \log D$.

3.8 Expectation values

We would like to find expectation values for observables in this formalism, which we need to make use of the variational method. Given some observable

$\mathcal{O} = \mathcal{O}_1 \otimes \cdots \otimes \mathcal{O}_n$ we compute its expectation value

$$\langle \mathcal{O} \rangle = \langle \psi_{MPS} | \mathcal{O} | \psi_{MPS} \rangle \quad (3.22)$$

$$= \sum_{\substack{k_1, \dots, k_n=1 \\ k'_1, \dots, k'_n=1}}^d \text{tr} \left(\prod_{m=1}^N A^{k_m^*} \right) \text{tr} \left(\prod_{m=1}^N A^{k'_m} \right) \left(\prod_{m=1}^N \langle k_m | \mathcal{O}_m | k'_m \rangle \right), \quad (3.23)$$

where we use the identity $\text{tr}(A \otimes B) = \text{tr} A \text{tr} B$ to write

$$= \text{tr} \left(\sum_{\substack{k_1, \dots, k_n=1 \\ k'_1, \dots, k'_n=1}}^d \prod_{m=1}^N A^{k_m^*} \otimes A^{k'_m} \langle k_m | \mathcal{O}_m | k'_m \rangle \right) \quad (3.24)$$

$$= \text{tr} \left(\prod_{m=1}^N \sum_{k_m, k'_m=1}^d A^{k_m^*} \otimes A^{k'_m} \langle k_m | \mathcal{O}_m | k'_m \rangle \right). \quad (3.25)$$

We define the scattering matrix as

$$E_{\mathcal{O}_m} := \sum_{k_m, k'_m=1}^d A^{k_m^*} \otimes A^{k'_m} \langle k_m | \mathcal{O}_m | k'_m \rangle. \quad (3.26)$$

This allows us to write our expectation values as a product over scattering matrices

$$\langle \mathcal{O} \rangle = \text{tr} \prod_{m=1}^N E_{\mathcal{O}_m}. \quad (3.27)$$

Specifically, E_1 is our first example of a transfer matrix, a concept that will become important for the continuum extension.

Chapter 4

Continuous Matrix Product States

4.1 Generic state

We begin by postulating the cMPS state. The physical system, we wish to describe is a quantum field and we provide an efficient, discrete “coordinate system” that naturally inherits many properties, most notably area laws, from its discrete cousin MPS. We consider a one-dimensional system of length L with periodic boundary conditions. The bosonic field is associated to field operators $\Psi(x)$ obeying a canonical commutation relation $[\Psi(x), \Psi^\dagger(y)] = \delta(x - y)$. The vacuum state $|\Omega\rangle$ associated to these operators is defined by $\Psi(x)|\Omega\rangle = 0$. Let Q and R be $D \times D$ matrices, which in general are position-dependent and called *auxiliary* variables. The cMPS state then is defined as

$$|\chi(Q, R)\rangle = \text{tr}_{aux} \left\{ B \mathcal{P} \exp \int_0^L ds Q(s) \otimes \mathbb{1} + R(s) \otimes \Psi^\dagger(s) \right\} |\Omega\rangle. \quad (4.1)$$

In the above expression, B encodes the boundary condition, which will not affect local physics and can be chosen as $B = \mathbb{1}$. We now proceed to explore the features of this class of states and provide physical justification for the particular structure.

4.2 Expansion in the field operators

Let us expand $|\chi\rangle$ in terms of field operators. Under the path-ordering the expansion yields

$$\begin{aligned} |\chi\rangle = \sum_{n=0}^{\infty} \int ds_1 \dots ds_n \text{tr} \{ & (\mathcal{P} e^{\int_0^{x_1} ds Q(s)}) R(x_1) (\mathcal{P} e^{\int_{x_1}^{x_2} ds Q(s)}) \dots \\ & \dots (\mathcal{P} e^{\int_{x_{n-1}}^{x_n} ds Q(s)}) R(x_n) (\mathcal{P} e^{\int_{x_n}^L ds Q(s)}) \} \Psi^\dagger(x_1) \dots \Psi^\dagger(x_n) |\Omega\rangle. \end{aligned} \quad (4.2)$$

We thus can interpret $\mathcal{P} e^{\int_a^b ds Q(s)}$ as a free propagation between points a and b . Furthermore the role of the $R(x)$ matrix is analogous to a scattering matrix at position x , that creates a field excitation (particle).

4.3 Derivation of cMPS as continuum limit of MPS

Continuous Matrix Product states were originally found as a continuum limit of MPS. In order to do that, we introduce a lattice with lattice spacing ϵ . Hence the continuum $[0, L]$ is approximated by a lattice of $N = L/\epsilon$ sites. Requiring that the resulting state has finite average particle number, [Verstraete and Cirac \[2010\]](#) found the limit

$$A^0 = \mathbb{1} + \epsilon Q \quad A^k = \frac{1}{k!} \epsilon^k R^k \quad (4.3)$$

with $D \times D$ matrices Q and R .

We now derive an expression for the norm of the cMPS state in this scheme by going into eqn. (3.25):

$$\langle \chi | \chi \rangle = \text{tr} \left(\prod_{m=1}^N \sum_{k_m, k'_m=1}^D A^{k_m*} \otimes A^{k'_m} \langle k_i | k'_m \rangle \right) \quad (4.4)$$

$$= \text{tr} \left(\prod_{m=1}^N \sum_{k_m} A^{k_m*} \otimes A^{k_m} \right) \quad (4.5)$$

$$= \text{tr} \prod_{m=1}^N (\mathbb{1} \otimes \mathbb{1} + \epsilon(Q \otimes \mathbb{1} + \mathbb{1} \otimes Q^* + R \otimes R^*) + \mathcal{O}(\epsilon^2)) \quad (4.6)$$

We let $N \rightarrow \infty$ while keeping $\epsilon = L/N$ fixed. In this limit, the above

expression goes to

$$\langle \chi | \chi \rangle = \text{tr} \exp [L(Q \otimes \mathbf{1} + \mathbf{1} \otimes Q^* + R \otimes R^*)] \quad (4.7)$$

In analogy to the transfer matrix for matrix product states we can identify the transfer matrix for continuous matrix product states as

$$T := Q \otimes \mathbf{1} + \mathbf{1} \otimes Q^* + R \otimes R^* \quad (4.8)$$

which lets us write the norm of the cMPS state compactly as $\langle \chi | \chi \rangle = \text{tr} \exp(LT)$

4.4 cMPS from continuous measurement

A second and more physical motivation for the form of $|\chi(Q, R)\rangle$ comes from the theory of continuous quantum measurement [Caves and Milburn, 1987]. We follow the original approach by Osborne et al. [2010] and introduce a *physical* system, which will function as our meter system and records the dynamics of a discrete quantum system. It is initialized in the ground state $|\Omega\rangle$ and we couple it to the discrete auxiliary system by evolving with the Hamiltonian

$$H(t) = K(t) \otimes \mathbf{1} + \sqrt{\epsilon} \sum_{k=1}^N \delta(t - k\epsilon) \left(iR(k\epsilon) \otimes a_{k\epsilon}^\dagger - iR^\dagger(k\epsilon) \otimes a_{k\epsilon} \right), \quad (4.9)$$

where $N\epsilon = L$ and $K(t)$ is the free Hamiltonian. We then go the standard way of integrating the Schrödinger equation, using the time-ordered exponential

$$U(0, L) = \mathcal{T} \exp \left(-i \int_0^L ds H(s) \right). \quad (4.10)$$

We sometimes abbreviate $U(0, L) = U(L)$. In the $\epsilon \rightarrow 0$ limit we can write the sum as an integral, integrate over the Dirac delta and taking $\Psi(k\epsilon) := a_{k\epsilon}/\sqrt{\epsilon}$ arrive at

$$H_{int}(t) = iR(t) \otimes \Psi^\dagger(t) - iR^\dagger(t) \otimes \Psi(t). \quad (4.11)$$

Thus, in the continuum limit the evolution operator reads

$$U(L) = \mathcal{T} \exp \left(\int_0^L ds (-iK(s)) \otimes \mathbf{1} + R(s) \otimes \Psi^\dagger(s) - R^\dagger(s) \otimes \Psi(s) \right). \quad (4.12)$$

If we initialize the meter system in the vacuum state $|\Omega\rangle$, we can reexpress $U(L)$ with the Zassenhaus formula and use that we act on the vacuum, i.e. $a|\Omega\rangle = 0$. We then have that

$$\begin{aligned} & \exp \left(\int_0^L ds -iK \otimes \mathbf{1} + R \otimes \Psi^\dagger \right) \exp \left(\int_0^L ds (-R^\dagger \otimes \Psi) \right) \times \\ & \exp \left(-\frac{1}{2} \int_0^L ds_1 \int_0^L ds_2 [-iK \otimes \mathbf{1} + R \otimes \Psi^\dagger, R^\dagger \otimes \Psi] \right) \exp(\text{higher orders}) |\Omega\rangle. \end{aligned} \quad (4.13)$$

Let us analyze the argument of the last term:

$$\begin{aligned}
& [-iK \otimes \mathbf{1} + R \otimes \Psi^\dagger, -R^\dagger \otimes \Psi] = \\
& i[K, R^\dagger] \otimes \Psi + R^\dagger R \otimes \Psi \Psi^\dagger - RR^\dagger \otimes \Psi^\dagger \Psi = \\
& i[K, R^\dagger] \otimes \Psi + R^\dagger R \otimes [\Psi, \Psi^\dagger] + [R, R^\dagger] \otimes \Psi^\dagger \Psi
\end{aligned} \tag{4.14}$$

Upon $\Psi |\Omega\rangle = 0$, $[\Psi(s_1), \Psi^\dagger(s_2)] = \delta(s_1 - s_2)$ and the Baker-Campbell-Hausdorff relation, we can recombine this to get

$$\exp \left(\int_0^L ds \left[-iK \otimes \mathbf{1} - \frac{1}{2} R^\dagger R \otimes \mathbf{1} + R \otimes \Psi^\dagger \right] \right) |\Omega\rangle. \tag{4.15}$$

Now defining $Q := -\frac{1}{2} R^\dagger R - iK$ and tracing out the auxiliary system, we again arrive at the standard form of a cMPS state

$$|\chi\rangle = \text{tr}_{\text{aux}} \mathcal{T} \exp \left(\int_0^L ds \left[Q(s) \otimes \mathbf{1} + R(s) \otimes \Psi^\dagger(s) \right] \right) |\Omega\rangle. \tag{4.16}$$

4.5 Expectation values in cMPS

It is possible to express expectation values entirely in terms of the auxiliary system, thus eliminating any dependence on the field system and converting to a *discrete* calculation. In general, expectation values of some observable \mathcal{O} localized in some spatial region are given by

$$\langle \mathcal{O} \rangle = \langle \chi | \mathcal{O} | \chi \rangle. \tag{4.17}$$

\mathcal{O} will usually consist of Ψ and its adjoint and its derivatives respectively, so

in order to evaluate eqn. (4.17) we want to commute these operators past $U(L)$, where they then annihilate the vacuum state via $\Psi|\Omega\rangle = 0$. To follow this idea, let us analyse the expression $\Psi|\chi\rangle = \Psi \text{tr}_{aux} U(L)|\Omega\rangle$ and expand the commutator $[\Psi(s), U(L)]$. To find an expression for this, let us start simple and recall the commutator product rule:

$$[A, BC] = B[A, C] + [A, B]C \quad (4.18)$$

To clear up notation, we define the n -th power commutator $C_n := [A, B^n]$. By iteratively using eqn. (4.18), we can generalize to an n -th power product rule:

$$\begin{aligned} C_n &= [A, B^n] = BC_{n-1} + C_1 B^{n-1} = \\ &= B^2 C_{n-2} + BC_1 B^{n-2} + C_1 B^{n-1} = \\ &= B^{n-1} C_1 + B^{n-2} C_1 B + \dots + BC_1 B^{n-2} + C_1 B^{n-1} \\ &= \sum_{k=0}^{n-1} B^{n-k-1} C_1 B^k \end{aligned} \quad (4.19)$$

In the continuum limit we obtain the following:

$$\begin{aligned} [\Psi(x), U(L)] &= \sum_{n=0}^{\infty} \int_{0 < y_1 < \dots < y_n < L} dy_1 \dots dy_n [\Psi(x), F(y_1) \dots F(y_n)] \\ &= \sum_{n=0}^{\infty} \sum_{k=0}^{n-1} \int dy_1 \dots dy_n F(y_1) \dots F(y_{n-k-1}) [\Psi(x), F(y_{n-k})] F(y_{n-k+1}) \dots F(y_n) \\ &= \int_0^L ds U(L-s) [\Psi(x), F(s)] U(s) \end{aligned}$$

With $F(s) = Q(s) \otimes \mathbb{1} + R(s) \otimes \Psi^\dagger(s)$ we find

$$\begin{aligned}
[\Psi(x), F(s)] &= [\mathbb{1} \otimes \Psi(x), Q(s) \otimes \mathbb{1} + R(s) \otimes \Psi^\dagger(s)] \\
&= R(s) \otimes \mathbb{1} \delta(x - s),
\end{aligned} \tag{4.20}$$

and therefore the commutator is

$$[\Psi(x), U(L)] = U(L - x)R(x)U(x) \tag{4.21}$$

where we omit trivial action on the respective spaces, since it is clear from the context that R really means $R \otimes \mathbb{1}$ and $\Psi(x)$ really means $\mathbb{1} \otimes \Psi(x)$.

We can hence eliminate the field operator and write

$$\begin{aligned}
\Psi(x) |\chi\rangle &= \text{tr} \Psi(x) U(L) |\Omega\rangle = \text{tr} \{ [\Psi(x), U(L)] |\Omega\rangle + U(L) \Psi(x) \} |\Omega\rangle \\
&= \text{tr} U(L - x) R(x) U(x) |\Omega\rangle
\end{aligned} \tag{4.22}$$

In order to evaluate derivatives of field operators, we can quite simply exchange the order of derivative and state, so we firstly do the cMPS substitution and only then apply the respective derivative, i.e.

$$\begin{aligned}
\left[\frac{d}{dx} \Psi(x), U(L) \right] &= \frac{d}{dx} [\Psi(x), U(L)] \\
&= U(L - x) [R, F] U(x) + U(L - x) R'(x) U(x)
\end{aligned} \tag{4.23}$$

where the last term vanishes for the translation invariant case, where we have $dR/dx = 0$. The commutator can be further simplified, since R commutes

with itself:

$$[R \otimes \mathbf{1}, Q \otimes \mathbf{1} + R \otimes \Psi^\dagger] = [R, Q] \quad (4.24)$$

4.6 Gauge freedom for cMPS

In the treatment of discrete matrix product states we established earlier that the transformation $A[n] \rightarrow X[n-1]A[n]X[n]^{-1}$ leaves the physical state unaffected. Let us analyse this freedom for the continuous case, where with lattice spacing ϵ we now define $g(x) = g(k\epsilon) := X[k]$ such that

$$A[k] \rightarrow g(k(\epsilon-1)) A[k] (g(k\epsilon))^{-1} \quad (4.25)$$

is a gauge transformation. With the continuum limit $A^0(x) = \mathbf{1} + \epsilon Q(x)$ and $A^1(x) = \epsilon R(x)$ this leads to a gauge transformation on Q and R of the following form:

$$A^0 \rightarrow g(x-\epsilon) A^0 g(x)^{-1} \quad (4.26)$$

Taylor-expanding $g(x-\epsilon) = g(x) - \epsilon \frac{dg}{dx} + \mathcal{O}(\epsilon^2)$ and evaluating everything at the same point x , this is equal to

$$\left(g - \epsilon \frac{dg}{dx}\right) (\mathbf{1} + \epsilon Q) g^{-1} = \mathbf{1} + \epsilon \left(g Q g^{-1} - \frac{dg}{dx} g^{-1}\right) + \mathcal{O}(\epsilon^2) \quad (4.27)$$

The gauge transformation on the auxiliary matrices thus reads

$$Q(x) \rightarrow g(x)Q(x)(g(x))^{-1} - \frac{dg(x)}{dx}(g(x))^{-1} \quad (4.28)$$

$$R(x) \rightarrow g(x)R(x)(g(x))^{-1} \quad (4.29)$$

4.7 Translation invariance

Throughout this thesis we will be concerned with translation invariant systems, such that the variational parameters (Q , R) become position-independent and their derivatives vanish. We may sometimes restore position dependence for illustration purposes.

4.8 The cMPS dictionary for expectation values

Collecting our rules for transforming field expressions to a description entirely written in terms of the discrete auxiliary system, we have:

$$\Psi(x) |\chi\rangle = \text{tr} U(L-x) R(x) U(x) |\Omega\rangle \quad (4.30)$$

$$\Psi'(x) |\chi\rangle = \text{tr} U(L-x) [R(x), Q(x)] U(x) |\Omega\rangle \quad (4.31)$$

$$T = \mathbf{1} \otimes Q^* + Q \otimes \mathbf{1} + R \otimes R^\dagger \quad (4.32)$$

$$\langle \chi | \chi \rangle = \exp(TL) \quad (4.33)$$

$$\langle \Psi^\dagger(x) \Psi(x) \rangle = \text{tr} \{ e^{TL} (R \otimes R^*) \} \quad (4.34)$$

$$\langle \partial_x \Psi^\dagger(x) \partial_x \Psi(x) \rangle = \text{tr} \{ e^{TL} [R, Q] \otimes [R, Q]^* \} \quad (4.35)$$

4.9 Useful isomorphisms

We can map our problem to a standard problem of dissipative dynamics by using the following isomorphism.¹ The isomorphism in its simplest form is just this:

$$|a\rangle\langle b| \Leftrightarrow |a\rangle \otimes |b\rangle \quad (4.36)$$

A corollary of this is that there is an isomorphism between linear operators on $\mathcal{H} \otimes \mathcal{H}$ and superoperators (operators acting on operators) on $\mathcal{B}(\mathcal{H})$:

$$\begin{aligned} A |a\rangle\langle b| B^\dagger &= \left(\sum_{ij} A_{ij} |i\rangle\langle j| \right) |a\rangle\langle b| \left(\sum_{mn} B_{mn}^* |n\rangle\langle m| \right) \\ &= \sum A_{ij} B_{mn}^* |i\rangle\langle j| |a\rangle\langle b| |n\rangle\langle m| \rightarrow \sum A_{ij} B_{mn}^* |i\rangle\langle j| |a\rangle\langle m| |n\rangle\langle b| \\ &= A \otimes B^* (|a\rangle \otimes |b\rangle) \end{aligned} \quad (4.37)$$

Hence the *standard isomorphism* reads

$$A |a\rangle\langle b| B^\dagger \Leftrightarrow A \otimes B^* |a\rangle\langle b| \quad (4.38)$$

We can extend it by linearity in the operators as well as in the states.

- Linearity in operators:

$$\sum_i A_i \otimes \bar{B}_i |a\rangle\langle b| \Leftrightarrow \sum_i A_i |a\rangle\langle b| B_i^\dagger \quad (4.39)$$

¹We have noticed some confusion in the literature regarding the name of this isomorphism. It should be distinguished from the Choi-Jamiołkowski Isomorphism relating channels to states.

- Linearity in states:

$$A \otimes \bar{B} \sum_{a,b} \Gamma_{ab} |a\rangle |b\rangle \leftrightarrow A \sum_{a,b} \Gamma_{ab} |a\rangle \langle b| B^\dagger \quad (4.40)$$

The right hand side of latter equation is already strongly reminiscent of a superoperator acting on a density matrix, if the matrix Γ_{ab} is chosen accordingly (i.e. positive and with unit trace) as

$$\sum_{a,b} \Gamma_{ab} |a\rangle \langle b| = \sum_{ab} \rho_{ab} |a\rangle \langle b| = \rho. \quad (4.41)$$

This density matrix ρ hence corresponds to a vector in $\mathcal{H} \otimes \mathcal{H}$ under the isomorphism:

$$|\rho\rangle := \sum_{ab} \rho_{ab} |a\rangle |b\rangle \quad (4.42)$$

4.10 Lindblad equation

Using the isomorphism gives a deep insight into the transfer matrix. Let us therefore analyse the action of the transfer matrix on $|\rho\rangle$, which is

$$\begin{aligned} T|\rho\rangle &= (Q \otimes \mathbb{1} + \mathbb{1} \otimes Q^* + R \otimes R^*) |\rho\rangle \\ &\Leftrightarrow Q\rho + \rho Q^\dagger + R\rho R^\dagger. \end{aligned} \quad (4.43)$$

Under the relation for Q , we found for the continuous measurement process

$$Q = -iK - \frac{1}{2}R^\dagger R \quad (4.44)$$

this superoperator is equal to

$$-i[K, \rho(x)] + R\rho(x)R^\dagger - \frac{1}{2}\{R^\dagger R, \rho(x)\} =: \mathcal{L}[\rho(x)]. \quad (4.45)$$

This is a master equation in the Lindblad form which describes dissipative dynamics of open quantum systems. If R was not present in the above equation, we would just have the Liouville-von Neumann equation describing the unitary evolution of the density matrix under the free Hamiltonian K . The coupling via the R -matrices introduces dissipation into the auxiliary system. The superoperator $\mathcal{L}[\rho] = \frac{d\rho}{dx}$ is called the Liouvillian and we thus have

$$\frac{d\rho}{dx} = -i[K, \rho] + R\rho R^\dagger - \frac{1}{2}\{R^\dagger R, \rho\}. \quad (4.46)$$

This Liouvillian has a unique steady state, for which $\mathcal{L}[\rho_{ss}] = 0$ holds, which will become important when we look at the thermodynamic limit.

For a bra acting on the transfer matrix from the left we get a similar relation, only that (Q, R) and (Q^\dagger, R^\dagger) change roles, such that

$$\langle \phi | T \Leftrightarrow Q^\dagger \phi + \phi Q + R^\dagger \phi R, \quad (4.47)$$

which leads to an analogous master equation in the Lindblad form.

4.11 Thermodynamic limit

In the thermodynamic limit $L \rightarrow \infty$ we can further simplify our equations. The matrix exponential of the transfer matrix $\exp(TL)$ will in this limit be dominated by its eigenvalue with the largest real part. If the latter is positive, we have a divergence for the thermodynamic limit. To avoid this, we must shift the transfer matrix exactly in such a way that its largest eigenvalue gets its real part shifted to zero. This comes down to a shift of Q . Let us call the largest eigenvalue $\lambda = \kappa + i\beta$. We then redefine $Q \rightarrow Q - \frac{1}{2}\kappa\mathbf{1}$. Suppose λ corresponded to an eigenvector $|r\rangle \in \mathcal{H} \otimes \mathcal{H}$. If we look at the Lindblad equation (4.45) of the virtual density matrix r (corresponding to $|r\rangle$ under the isomorphism), we also see that the imaginary part β must be zero. Therefore we have one eigenvalue zero and all other eigenvalues have negative real part and decay in the thermodynamic limit. Let us call the left eigenvector $\langle l|$ and normalize such that $\langle l|r\rangle = 1$. We then see that $P_0 := |l\rangle\langle r|$ forms the projector into the zero-eigenspace, since

$$(P_0)^2 = |r\rangle\langle l|r\rangle\langle l| = |r\rangle\langle l|. \quad (4.48)$$

Hence for the thermodynamic limit we get

$$\lim_{N \rightarrow \infty} \exp(TL) = |r\rangle\langle l|. \quad (4.49)$$

A useful corollary of this is, that our cMPS state is now automatically normalized, as $\langle \chi|\chi\rangle = \text{tr} \exp(TL) = \langle l|r\rangle = 1$.

4.12 Steady state for expectation values

Under the isomorphism, $|r\rangle$ and $\langle l|$ are associated to *virtual density operators* for the auxiliary system, which we simply denote r and l , and in general are subject to the dissipative evolution governed by the above Liouvillian. We can exploit the description in terms of dissipative dynamics to determine $|r\rangle$ and $\langle l|$, since they correspond to steady states (and hence eigenvalue zero) under the isomorphism. Under a gauge transformation we can find out how they transform by looking at the transformation behaviour of T , which is

$$\begin{aligned} \langle l|T|r\rangle &\rightarrow \langle l'|\mathbb{1} \otimes g^*Q^*(g^{-1})^* + gQg^{-1} \otimes \mathbb{1} + gRg^{-1} \otimes g^*R^*(g^{-1})^* |r'\rangle \\ &= \langle l'|(g \otimes g^*)T(g^{-1} \otimes (g^{-1})^*) |r'\rangle. \end{aligned} \quad (4.50)$$

We therefore require that under a gauge transformation $|r'\rangle = g \otimes g^* |r\rangle$ and $\langle l'| = \langle l|g^{-1} \otimes (g^{-1})^*$, which under the isomorphism translates to

$$r \rightarrow grg^\dagger \quad l \rightarrow (g^{-1})^\dagger lg^{-1}. \quad (4.51)$$

We can now shift the whole evolution into only one of the density matrices by exploiting the above gauge freedom in the following manner. We do the gauge transformation $g(x) = \sqrt{l(x)}$, which leads to a new l via $\tilde{l}(x) = \left(\sqrt{l(x)^\dagger}\right)^{-1} l(x) \left(\sqrt{l(x)}\right)^{-1} = \mathbb{1}_D$, which under the above described evolution

$$\frac{d}{dx}l(x) = Q^\dagger l + lQ + R^\dagger lR \quad (4.52)$$

now remains constant, because for $l = \mathbb{1}$ this evolution is

$$Q^\dagger + Q + R^\dagger R = 0, \quad (4.53)$$

which is zero due to $Q = -iK - \frac{1}{2}R^\dagger R$. We have thus “shifted” the entire evolution into r , which evolves according to the Lindblad equation. It has a unique steady state solution ρ_{ss} . We can therefore make the substitution

$$\text{tr}(A \otimes B^* |r\rangle \langle l|) \underset{\text{isomorphism}}{\Leftrightarrow} \text{tr}(Ar \cdot lB^\dagger) \underset{\text{gauge freedom}}{\rightarrow} \text{tr}(B^\dagger A \rho_{ss}). \quad (4.54)$$

So using the isomorphism and the steady state ρ_{ss} to simplify the expectation values given in section (4.8) in the thermodynamic limit, we get the following collection:

$$\langle \Psi^\dagger(x) \Psi(x) \rangle = \text{tr}(R^\dagger R \rho_{ss}) \quad (4.55)$$

$$\left\langle \frac{d\Psi^\dagger}{dx} \frac{d\Psi}{dx} \right\rangle = \text{tr}([Q, R]^\dagger [Q, R] \rho_{ss}) \quad (4.56)$$

$$\langle \Psi^\dagger \Psi^\dagger \Psi \Psi \rangle = \text{tr}((R^\dagger)^2 R^2 \rho_{ss}). \quad (4.57)$$

Finding the steady-state of a Lindbladian is a standard problem in quantum optics and hence there are tools readily available to find them for a given problem. We use the `quantum optics toolbox` [Tan, 2002] in MATLAB, which allows us to define superoperators and find the steady state by an inverse power method with random initial conditions.

Chapter 5

The Lieb-Liniger model

The model of a one-dimensional gas satisfying Bose-Einstein statistics is named after Lieb and Liniger, who were the first to solve it [Lieb and Liniger, 1963]. Using the Bethe ansatz they were able to come up with an exact solution of the model, which was in accordance with previous approximations like Bogoliubov's theory. In recent years the Lieb-Liniger model has attracted renewed attention after it has become experimentally conceivable to realize gases with effectively one-dimensional Lieb-Liniger-like behaviour [Seiringer and Yin, 2007]. From our perspective, the model will serve as a play-ground for understanding the cMPS procedure and comparing it to the solution by Lieb and Liniger, as was done by Verstraete and Cirac [2010]

5.1 Lieb-Liniger Hamiltonian

Let us define the Lieb-Liniger Hamiltonian via the non-relativistic boson gas with ultra-local interactions governed by the interaction parameter c

$$H = - \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{1 \leq i < j \leq N} \delta(x_i - x_j). \quad (5.1)$$

After second quantization we arrive at the full Lieb-Liniger field Hamiltonian:

$$H = \left(\int_{-\infty}^{\infty} dx \frac{d\psi^\dagger(x)}{dx} \frac{d\psi(x)}{dx} + c\psi^\dagger(x)\psi^\dagger(x)\psi(x)\psi(x) \right). \quad (5.2)$$

5.2 Ground state

Our principal goal will be to find the ground state energy as a function of the interaction parameter c . We will use the variational method by expressing the energy expectation value in the cMPS formalism. We then seed a random configuration of auxiliary fields and feed it into a minimization algorithm, which searches for the configuration of auxiliary fields with the minimal energy expectation value. We will find that the final configuration will be independent on the initial seed, which indicates a strong convergence of the used method.

5.3 Tonks-Girardeau limit

In the limit of infinite repulsion $c \rightarrow \infty$ it has been shown [Lieb and Liniger, 1963] that the ground state energy goes to

$$\lim_{c \rightarrow \infty} E(c) = \frac{\pi^2}{3}. \quad (5.3)$$

An interesting aside to this particular limit is that this limit can be identified with a fermionic model due to the fact that infinite repulsion is analogous to the Paul exclusion principle.

5.4 Number operator

The number operator is given by

$$\hat{N} = \int dx \Psi^\dagger(x) \Psi(x) \quad (5.4)$$

and can be seen to commute with the full Hamiltonian, as

$$\begin{aligned}
[N, H] &= \int dx dy \left[\Psi^\dagger(x) \Psi(x), \partial_y \Psi^\dagger(y) \partial_y \Psi(y) + \Psi^\dagger(y) \Psi^\dagger(y) \Psi(y) \Psi(y) \right] \\
&= \int dx dy \Psi^\dagger(x) \left[\Psi(x), \partial_y \Psi^\dagger(y) \partial_y \Psi(y) \right] + \left[\Psi^\dagger(x), \partial_y \Psi^\dagger(y) \partial_y \Psi(y) \right] \Psi(x) \\
&+ \Psi^\dagger(x) \left[\Psi(x), \Psi^\dagger(y) \Psi^\dagger(y) \right] \Psi(y) \Psi(y) + \Psi^\dagger(y) \Psi^\dagger(y) \left[\Psi^\dagger(x), \Psi(y) \Psi(y) \right] \Psi(x) \\
&= \int dx dy \left[-\partial_y \Psi^\dagger(y) \delta(x-y) \partial_y \Psi(y) + \partial_y \Psi^\dagger(y) \delta(x-y) \partial_y \Psi(y) \right. \\
&\quad \left. + \Psi^\dagger(x) 2\delta(x-y) \Psi^\dagger(y) \Psi(y) \Psi(y) + \Psi^\dagger(y) \Psi^\dagger(y) (-2\delta(x-y) \Psi(y)) \Psi(x) \right] \\
&= 0.
\end{aligned} \tag{5.5}$$

It is therefore a conserved quantity. We incorporate this requirement by fixing the particle number. In the cMPS formalism this constraint amounts to fixing

$$\langle \Psi^\dagger \Psi \rangle = \text{tr} [R^\dagger R \rho_{ss}] = \text{const.}, \tag{5.6}$$

which we will set equal to one in our numerical implementation.

5.5 Minimization

We use the constrained minimization routine `fmincon` in MATLAB, which we initialize with random matrices. The code can be found in the appendix to this thesis. We then sweep through an interval of interaction parameters c . We get the following results (see figure (5.1)):

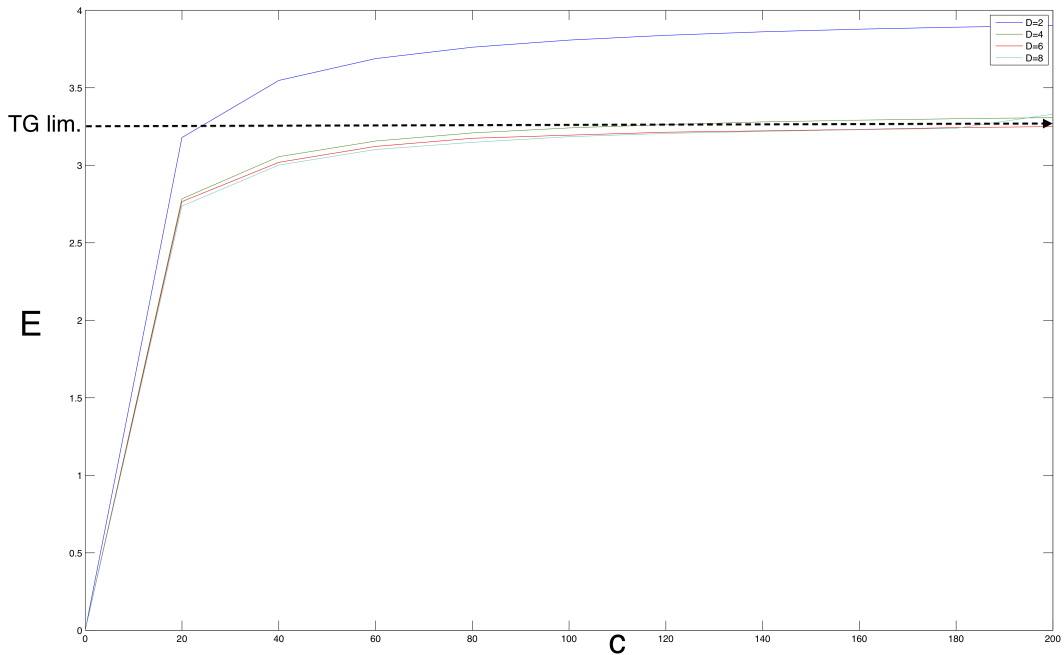


Figure 5.1: Energy density E against interaction parameter c for the Lieb-Liniger model, from top to bottom: $D = 2, 4, 6, 8$. Black horizontal line: $\pi^2/3$, the Tonks-Girardeau limit for $c \rightarrow \infty$

Analyzing the plot in figure (5.1) we note that while there is a significant difference between the result for $D = 2$ and $D = 4$, the results for higher bond dimensions are very close to one another, which is a good indication that we are converging towards the correct solution. This is corroborated by approaching the correct large c asymptotic behaviour and it has been shown that the solution for moderate bond dimension is virtually indistinguishable from the exact solution obtained by the Bethe ansatz. We thus have shown that the cMPS formalism is capable of capturing the relevant physics with very moderate bond dimensions, which is further supported in the next chapter by studying the Dirac model.

Chapter 6

Free Dirac model

The Dirac equation was formulated in 1928 by Paul Dirac and can certainly be viewed as one of the great triumphs of theoretical physics, most notably predicting the existence of anti-particles, which were experimentally confirmed in 1932 by Anderson. The modern perspective on the quantized Dirac equation provides a positive definite Hamiltonian in terms of its particle and antiparticle content, which is related to the technique of normal ordering. However, we would like to illustrate certain features of the cMPS formalism for which we will follow a direct analysis in terms of positive and negative energy modes. In this setting, we expect a naïve variational calculation of the ground state to fail due to unbounded high-momentum physics dominating over the low energy behaviour. To remedy this, we introduce a high-momentum cutoff and analyse the benefit of the cMPS parametrization, which guarantees a p^{-4} limiting behaviour at large momenta. This allows a meaningful extraction of physics, in which we describe Dirac's historical resolution of the Dirac sea and illustrate the natural effectiveness of cMPS with

regulators.

6.1 Dirac equation

The most compact way to write down the free Dirac equation is

$$(i\gamma^\mu \partial_\mu - m)\Psi = 0, \quad (6.1)$$

where Ψ is a two-component spinor, as we are in $1 + 1$ dimensions. We thus need the two gamma-matrices γ^0 and γ^1 , which obey the Clifford-algebra

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}\mathbb{1} \quad (6.2)$$

and where we make the choice $\gamma^0 = \sigma_z$ and $\gamma^1 = i\sigma_x$.

6.2 Lagrangian and Hamiltonian

The Lagrangian that has the Dirac equation as its equation of motion is

$$\mathcal{L} = \bar{\Psi}(i\gamma^\mu \partial_\mu - m)\Psi, \quad (6.3)$$

where the Dirac conjugate of Ψ is defined as $\bar{\Psi} := \Psi^\dagger \gamma^0$. The Hamiltonian can be found as the Legendre transform of \mathcal{L} and is therefore

$$\mathcal{H} = (\partial_0 \bar{\Psi}) \frac{\partial \mathcal{L}}{\partial (\partial_0 \bar{\Psi})} + \frac{\partial \mathcal{L}}{\partial (\partial_0 \Psi)} (\partial_0 \Psi) - \mathcal{L} \quad (6.4)$$

$$= \bar{\Psi} i \gamma^0 \partial_0 \Psi - \mathcal{L} = \bar{\Psi} i \gamma^1 \frac{d}{dx} \Psi + m \bar{\Psi} \Psi. \quad (6.5)$$

We thus arrive at the following Dirac Hamiltonian

$$\mathcal{H} = \Psi_2^\dagger \frac{\partial \Psi_1}{\partial x} - \Psi_1^\dagger \frac{\partial \Psi_2}{\partial x} + m(\Psi_1^\dagger \Psi_1 - \Psi_2^\dagger \Psi_2). \quad (6.6)$$

6.3 cMPS for multiple particle species

In our cMPS treatment up to now we were only concerned with one particle species (bosons). Since we now want to study the Dirac model, which has two fermions involved, let us show how the generalisation is made. The end result here will be that the variables for the auxiliary system must obey the same statistics as their physical field counterparts. This follows in particular from requiring regularity of the cMPS state kinetic energy. The fields now carry an index Ψ_α and so do their auxiliary interaction terms R_α . The generalized cMPS thus reads

$$|\chi(Q, R_\alpha)\rangle = \text{tr } B \mathcal{P} \exp \int_0^L ds Q(s) \otimes \mathbf{1} + \sum_\alpha R_\alpha \otimes \Psi_\alpha^\dagger(x) |\Omega\rangle \quad (6.7)$$

and the transfer matrix is generalized in a straightforward manner to

$$T = Q \otimes \mathbf{1} + \mathbf{1} \otimes Q^* + \sum_\alpha R_\alpha \otimes R_\alpha^*. \quad (6.8)$$

We now allow the fields to be either fermionic or bosonic, i.e. they obey commutation or anticommutation relations:

$$[\Psi_\alpha(x), \Psi_\alpha^\dagger(y)] = \delta(x - y) \quad \text{bosonic}, \quad (6.9)$$

$$\{\Psi_\alpha(x), \Psi_\alpha^\dagger(y)\} = \delta(x - y) \quad \text{fermionic}. \quad (6.10)$$

In the following we will however only be concerned with fermions.

6.4 Picking up a minus sign

To compute expectation values of field operators, we want to arrive at the analogue of eqn. (4.21), where we computed the commutator of the field operator with the evolution operator $U(L)$. The difference is that we now pick up an additional sign, when we commute fermionic fields past another. We therefore define the notation for this sign-property via

$$\begin{aligned} s_\alpha &= 0 \quad (\alpha \text{ bosonic}), \\ s_\alpha &= 1 \quad (\alpha \text{ fermionic}), \end{aligned} \quad (6.11)$$

and define generalized evolution operators $\{U_{s_\alpha}(x, y)\}$ as

$$U_{s_\alpha}(x, y) := \mathcal{P} \exp \int_x^y dz Q(z) \otimes \mathbb{1} + \sum_\beta (-1)^{s_\alpha s_\beta} R_\beta(z) \otimes \psi_\beta^\dagger(z). \quad (6.12)$$

We emphasize that $(-1)^{s_\alpha s_\beta}$ is -1 if and only if α and β are both fermionic and $+1$ otherwise. Furthermore we define the transfer matrix T_{s_α} as

$$T_{s_\alpha} := Q \otimes \mathbb{1} + \mathbb{1} \otimes Q^* + \sum_{\alpha} (-1)^{s_\alpha} R_\alpha \otimes R_\alpha^*. \quad (6.13)$$

We find that

$$[\Psi_\alpha(x), U(L)] = U_{s_\alpha}(0, x) R_\alpha(x) U(x, L). \quad (6.14)$$

We also want to look at the derivative, whose analysis follows the same manner as before but becomes a bit more involved due keeping track of the s_α :

$$\begin{aligned} \frac{d}{dx} \Psi_\alpha(x) |\chi\rangle &= \frac{d}{dx} \text{tr} B U_{s_\alpha}(0, x) R_\alpha(x) U(x, L) |\Omega\rangle \\ &= \text{tr} B \left\{ \frac{dU_{s_\alpha}(0, x)}{dx} R_\alpha(x) U(x, L) + U_{s_\alpha}(0, x) \frac{dR_\alpha(x)}{dx} U(x, L) \right. \\ &\quad \left. + U_{s_\alpha}(0, x) R_\alpha(x) \frac{dU(x, L)}{dx} \right\} |\Omega\rangle. \end{aligned} \quad (6.15)$$

From the definition of the evolution operator, its derivative just brings down its argument and we get

$$\begin{aligned} \frac{d}{dx} U_{s_\alpha}(0, x) &= U_{s_\alpha}(0, x) \left(Q(x) \otimes \mathbb{1} + \sum_{\beta} (-1)^{s_\alpha s_\beta} R_\beta(x) \otimes \Psi_\beta^\dagger(x) \right) \\ \frac{d}{dx} U(x, L) &= - \left(Q(x) \otimes \mathbb{1} + \sum_{\beta} R_\beta(x) \otimes \Psi_\beta^\dagger(x) \right) U(x, L), \end{aligned} \quad (6.16)$$

such that we find that

$$\begin{aligned} \frac{d}{dx} \Psi_\alpha(x) |\chi\rangle &= \text{tr } U_{s_\alpha}(0, x) \left\{ [Q(x), R_\alpha(x)] \otimes \mathbf{1} + \frac{dR_\alpha(x)}{dx} \right. \\ &+ \left. \sum_\beta [(-1)^{s_\alpha s_\beta} R_\beta(x) R_\alpha(x) - R_\alpha(x) R_\beta(x)] \otimes \Psi_\beta^\dagger(x) \right\} U(x, L) |\chi\rangle. \end{aligned} \quad (6.17)$$

The first two terms inside the curly brackets are familiar from the single boson case but we have picked up a new term which now encodes the particle statistics. Looking at the norm of the state, it should make us worry that acting with Ψ_α on the cMPS state now gave us a contribution including Ψ_α^\dagger . This renders the state non-normalizable, unless we fix the corresponding auxiliary matrices such that this term vanishes. We thus require

$$(-1)^{s_\alpha s_\beta} R_\beta(x) R_\alpha(x) - R_\alpha(x) R_\beta(x) = 0. \quad (6.18)$$

which is to say, the auxiliary interaction terms must obey the same statistics as their physical counterparts. Let us note that this is consistent with the single boson case since matrices trivially commute with themselves. In contrast to that, we now need discrete anticommuting matrices to accommodate the Dirac fermions. Following [Haegeman \[2011\]](#), we now use a construction by Jordan and Wigner, where we dedicate a $\mathbb{C}^2 \otimes \mathbb{C}^2$ subspace to the construction of anticommuting matrices.

6.5 Jordan-Wigner transformation

In order to construct anticommuting matrices $\{R_\alpha, R_\beta\} = 0$ we enforce anticommutativity on the $\mathbb{C}^2 \otimes \mathbb{C}^2$ subspace. This construction is due to [Jor-](#)

dan and Wigner [1928], who originally introduced it to map spin systems to fermionic systems. We parametrize the R_α matrices (no summation) as:

$$R_\alpha = c_\alpha \otimes \tilde{R}_\alpha \quad (6.19)$$

and then use the Jordan-Wigner transformation in the construction of the c_α as

$$c_n = \left(\bigotimes_{k < n} \sigma_k^z \right) \otimes \sigma_n^- \quad (6.20)$$

with the lowering operator $\sigma^- = |0\rangle\langle 1|$ and the trivial action on other sites suppressed. Hence for our model we have

$$c_1 = \sigma_1^- = \sigma^- \otimes \mathbb{1} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (6.21)$$

$$c_2 = \sigma_1^z \otimes \sigma_2^- = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (6.22)$$

For the anticommutativity to carry through to the R_α matrices on the full space, we must require $[\tilde{R}_\alpha, \tilde{R}_\beta] = 0$. We provide this by choosing \tilde{R}_α diagonal.

$$\tilde{R}_\alpha = \text{diag}(r_1, \dots, r_D), \quad (6.23)$$

where we defined \tilde{D} as the dimension of the remaining subspace, such that $D = 4\tilde{D}$. The complete parametrisation (eqn. 6.19) then reads

$$R_1 = \begin{pmatrix} 0 & 0 & \tilde{R}_1 & 0 \\ 0 & 0 & 0 & \tilde{R}_1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad R_2 = \begin{pmatrix} 0 & \tilde{R}_2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\tilde{R}_2 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (6.24)$$

which indeed manifestly ensures nilpotency and anticommutativity.

6.6 Expectation values

With the regularity properties now established, the cMPS substitution rules are analogous to the rules given in section (4.8). Thus, evaluating the expectation value of the Dirac Hamiltonian in this manner leads us to the following expression

$$\begin{aligned} \langle \chi | \mathcal{H} | \chi \rangle &= \langle \chi | \Psi_2^\dagger \frac{\partial \Psi_1}{\partial x} - \Psi_1^\dagger \frac{\partial \Psi_2}{\partial x} + m(\Psi_1^\dagger \Psi_1 - \Psi_2^\dagger \Psi_2) | \chi \rangle = \\ &\text{tr} \left\{ ([Q, R_1] \otimes R_2^* - [Q, R_2] \otimes R_1^* + mR_1 \otimes R_1^* - mR_2 \otimes R_2^*) e^{TL} \right\} \end{aligned} \quad (6.25)$$

over the variational manifold parametrized by (Q, R_1, R_2) .

6.7 Solution of the quantized Dirac equation

We briefly recall the standard theory for solving the Dirac equation [Peskin and Schroeder, 1995]. We introduce two fermionic ladder operators obey-

ing anti-commutation relations $\{a_{k_1}, a_{k_2}^\dagger\} = 2\pi\delta(k_1 - k_2)$ and $\{b_{k_1}^\dagger, b_{k_2}\} = 2\pi\delta(k_1 - k_2)$. With the two-component basis spinors u and v we recall the solution to the quantized Dirac equation

$$\psi(x) = \int \frac{dk}{2\pi} \frac{1}{\sqrt{2E_k}} \left(u(k)a_k e^{-ikx} + v(k)b_k^\dagger e^{ikx} \right). \quad (6.26)$$

In momentum space with $E_k = \sqrt{k^2 + m^2}$ and $k^\mu = (E_k, k)$ we have

$$(\gamma^\mu k_\mu - m)u = 0 \quad (6.27)$$

$$(E_k \sigma^z - ik \sigma^x - m \mathbf{1})u = 0 \quad (6.28)$$

$$\begin{pmatrix} E_k - m & -ik \\ -ik & -E_k - m \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = 0 \quad (6.29)$$

$$(E_k - m)u_1 = ik u_2 \quad (6.30)$$

$$(E_k + m)u_2 = ik u_1 \quad (6.31)$$

Hence we get u and v with parameters λ and $\tilde{\lambda}$:

$$u = \lambda \begin{pmatrix} i(E_k + m) \\ k \end{pmatrix} \quad v = \tilde{\lambda} \begin{pmatrix} ik \\ E_k + m \end{pmatrix} \quad (6.32)$$

We follow the convention for the normalization of u and v [Peskin and Schroeder, 1995]

$$u^\dagger u = 2E_k \quad v^\dagger v = 2E_k \quad (6.33)$$

which fixes λ and $\tilde{\lambda}$, such that we have

$$u = \frac{1}{\sqrt{E_k + m}} \begin{pmatrix} E_k + m \\ -ik \end{pmatrix} \quad (6.34)$$

$$v = \frac{1}{\sqrt{E_k + m}} \begin{pmatrix} ik \\ E_k + m \end{pmatrix}. \quad (6.35)$$

We thus have found the solution to equation (6.26). We now “invert” it to get expressions for the creation and annihilation operators:

$$a_k = \frac{E_k + m}{\sqrt{2E_k(E_k + m)}} \Psi_1(k) + \frac{ik}{\sqrt{2E_k(E_k + m)}} \Psi_2(k) \quad (6.36)$$

$$b_{-k}^\dagger = \frac{ik}{\sqrt{2E_k(E_k + m)}} \Psi_1(k) + \frac{m + E_k}{2E_k(E_k + m)} \Psi_2(k). \quad (6.37)$$

6.8 Momentum space occupation-number

To study the behaviour of the cMPS formalism in the relativistic case of the free Dirac field we look at the occupation number in momentum space. The goal is to try to reproduce the filling of the Dirac sea for negative energy solutions and no filling for positive energy solutions, which was found by [Haege-
man et al. \[2010\]](#). The two-point function $c_{\alpha,\beta}(x, y) = \langle \chi | \psi_\alpha^\dagger(x) \psi_\beta(y) | \chi \rangle$ in real space is readily expressed in the cMPS formalism as

$$\begin{aligned} c_{\alpha,\beta}(x, y) &= \langle \chi | \psi_\alpha^\dagger(x) \psi_\beta(y) | \chi \rangle \\ &= \Theta(x - y) \langle l | (R_\beta \otimes \mathbf{1}) e^{T_{s_\alpha}(x-y)} (\mathbf{1} \otimes R_\alpha^*) | r \rangle \\ &\quad + \Theta(y - x) \langle l | (\mathbf{1} \otimes R_\alpha^*) e^{T_{s_\alpha}(y-x)} (R_\beta \otimes \mathbf{1}) | r \rangle. \end{aligned} \quad (6.38)$$

Note that, as expected, this only depends on the relative distance $y - x$. We therefore can define $z = x - y$ and hence

$$\begin{aligned} c_{\alpha,\beta}(z) &= \Theta(z) \langle l | (R_\beta \otimes \mathbf{1}) e^{T_{s_\alpha} z} (\mathbf{1} \otimes R_\alpha^*) | r \rangle \\ &\quad + \Theta(-z) \langle l | (\mathbf{1} \otimes R_\alpha^*) e^{-T_{s_\alpha} z} (R_\beta \otimes \mathbf{1}) | r \rangle. \end{aligned} \quad (6.39)$$

We now define momentum occupation as

$$n_{\alpha\beta}(p, q) = \langle \chi | \psi_\alpha^\dagger(p) \psi_\beta(q) | \chi \rangle \quad (6.40)$$

with the Fourier transformed operators

$$\tilde{\psi}_\alpha(p) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ipx} \psi_\alpha(x). \quad (6.41)$$

Since we have that

$$\begin{aligned}
n_{\alpha\beta}(p, q) &= \int \frac{dx dy}{2\pi} e^{ipx - iqy} c_{\alpha\beta}(x, y) \\
&= \int \frac{dx dy}{2\pi} e^{ipx - iqy} \{ \Theta(x - y) \langle l | (R_\beta \otimes \mathbf{1}) e^{T_{s_\alpha}(x-y)} (\mathbf{1} \otimes R_\alpha^*) | r \rangle \\
&\quad + \Theta(y - x) \langle l | (\mathbf{1} \otimes R_\alpha^*) e^{T_{s_\alpha}(y-x)} (R_\beta \otimes \mathbf{1}) | r \rangle \}, \tag{6.42}
\end{aligned}$$

we change coordinates to $u = x - y$ and $w = x + y$. The Jacobian is $\det J = \frac{1}{2}$, such that the measure changes as $dx dy = du dw/2$. Expressing the old in the new coordinates gives $x = (u + w)/2$ and $y = (w - u)/2$ and the argument of the exponential is $i(px - qy) = i(p(u + w) - q(w - u))/2 = iu(p + q)/2 + iw(p - q)/2$. Since the integrand depends only on u , we can integrate out w , which gives

$$\int \frac{dw}{2\sqrt{2\pi}} e^{i(p-q)w/2} = \delta(p - q). \tag{6.43}$$

This enforces $p = q$ and hence

$$\begin{aligned}
n_{\alpha\beta}(p, q) &= \delta(p - q) \int \frac{du}{\sqrt{2\pi}} e^{iup} \Theta(u) \langle l | (R_\beta \otimes \mathbf{1}) e^{T_{s_\alpha}u} (\mathbf{1} \otimes R_\alpha^*) | r \rangle \\
&\quad + \Theta(-u) \langle l | (\mathbf{1} \otimes R_\alpha^*) e^{-T_{s_\alpha}u} (R_\beta \otimes \mathbf{1}) | r \rangle. \tag{6.44}
\end{aligned}$$

We integrate (the Heaviside step-functions change the ranges of integration), using the same argument as in discussion for the thermodynamic limit (sec-

tion 4.11), which guarantees that the integrand falls off at infinity.

$$\begin{aligned} \int_0^\infty du \exp(u(ip\mathbf{1} + T_{s_\alpha})) &= -(ip\mathbf{1} + T_{s_\alpha})^{-1} \\ \int_{-\infty}^0 du \exp(u(ip\mathbf{1} - T_{s_\alpha})) &= (ip\mathbf{1} - T_{s_\alpha})^{-1} \end{aligned} \quad (6.45)$$

Summing up, we now have the following relation for the number density

$$\begin{aligned} n_{\alpha\beta}(p, q) &= \delta(p - q) \left(-\langle l | (R_\beta \otimes \mathbf{1}) (ip\mathbf{1} + T_{s_\alpha})^{-1} (\mathbf{1} \otimes R_\alpha^*) | r \rangle \right. \\ &\quad \left. + \langle l | (\mathbf{1} \otimes R_\alpha^*) (ip\mathbf{1} - T_{s_\alpha})^{-1} (R_\beta \otimes \mathbf{1}) | r \rangle \right) \quad (6.46) \\ &=: \delta(p - q) n_{\alpha\beta}(p). \end{aligned}$$

6.9 Large momentum behaviour

We can deduce the large-momentum behaviour of $n_{\alpha\beta}$ by noting that the second derivative of its counterpart in real space $c_{\alpha\beta}$ is equivalent to the kinetic energy, for which we derived the regularity properties in section (6.4) and which has led us to require $\{R_\alpha, R_\beta\} = 0$ (equation 6.18). We therefore know that the second derivative $\frac{d^2}{dx^2} c_{\alpha\beta}(x)$ of the number density must be continuous, specifically at $x = 0$. Let us relate this to the momentum space picture

$$\begin{aligned} c_{\alpha\beta}(x) &= \int \frac{dp}{\sqrt{2\pi}} e^{-ipx} n_{\alpha\beta}(p) \\ \Rightarrow \frac{d^2}{dx^2} c_{\alpha\beta}(x) &= \frac{d^2}{dx^2} \int \frac{dp}{\sqrt{2\pi}} e^{-ipx} n_{\alpha\beta}(p) \quad (6.47) \\ &\Rightarrow \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi}} e^{-ipx} p^2 n_{\alpha\beta}(p). \end{aligned}$$

This tells us that due to the continuity at $x = 0$ and the requirement that this integral exists, the large momentum behaviour of $n(p)$ has to fall off at least like

$$n_{\alpha\beta}(p) \sim p^{-4}. \quad (6.48)$$

6.10 Scale transformations

We have shown how large momenta are suppressed in our construction of the cMPS matrices. There does however remain a problem related to the negative energy solutions of the Dirac equation. If we have a configuration of Q and R_α related to this negative energy, the variational method will push this solution to become arbitrarily negatively large by the rescaling freedom $Q \rightarrow cQ$ and $R \rightarrow \sqrt{c}R$, which rescales the transfer matrix $T \rightarrow cT$ and therefore leaves eigenvalue zero of T and thus also $|r\rangle$ and $\langle l|$ unchanged. In the same manner it also rescales the sign-flipped transfer matrix $T_{s_\alpha} \rightarrow cT_{s_\alpha}$. The momentum occupation under the rescaling behaves like this:

$$\begin{aligned} n_{\alpha\beta}(p) &= \left(-\langle l| (R_\beta \otimes \mathbf{1}) (ip\mathbf{1} + T_{s_\alpha})^{-1} (\mathbf{1} \otimes R_\alpha^*) |r\rangle + \text{conjugate term} \right) \\ &\xRightarrow[\substack{R_\alpha \rightarrow \sqrt{c}R_\alpha \\ T_{s_\alpha} \rightarrow cT_{s_\alpha}}]{\quad} \left(-\langle l| (R_\beta \otimes \mathbf{1}) \sqrt{c}(ip\mathbf{1} + cT_{s_\alpha})^{-1} \sqrt{c}(\mathbf{1} \otimes R_\alpha^*) |r\rangle + \text{conj.} \right) \end{aligned} \quad (6.49)$$

and with

$$c(ip\mathbf{1} \pm cT_{s_\alpha})^{-1} = \left(i\frac{p}{c}\mathbf{1} \pm T_{s_\alpha} \right)^{-1} \quad (6.50)$$

this tells us that

$$n_{\alpha\beta}(p) \xrightarrow[\begin{smallmatrix} R_\alpha \rightarrow \sqrt{c}R_\alpha \\ T_{s\alpha} \rightarrow cT_{s\alpha} \end{smallmatrix}]{\Rightarrow} n_{\alpha\beta}(p/c). \quad (6.51)$$

Let us analyse what this means for our momentum occupation. Suppose the p^{-4} fall-off for some configuration of (Q, R_α) happened at momentum $p = \Lambda$, which implies that $n_{\alpha\beta}(p/\Lambda)$ drops to zero at Λ . The variational method then pushes for a rescaling as described above, which leads to $n_{\alpha\beta}(p/(c\Lambda))$ and hence the drop to zero in the number density is pushed away to arbitrarily large momenta.

6.11 Regularisation

In order to fix this pushing behaviour we introduce the cutoff term proposed by [Haegeman et al. \[2010\]](#) $\frac{1}{\Lambda} \frac{d\Psi^\dagger}{dx} \frac{d\Psi}{dx}$. This term constrains the negative energy solutions to a finite region. In momentum space, the upper limit to this region is given by

$$\begin{aligned} \sqrt{p^2 + m^2} = p^2/\Lambda &\Leftrightarrow p_{\text{cutoff}} = \Lambda \sqrt{\frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4m^2}{\Lambda^2}}} \\ p_{\text{cutoff}} &= \Lambda + \mathcal{O}\left(\frac{m^2}{\Lambda^2}\right). \end{aligned} \quad (6.52)$$

We therefore expect the cutoff to happen at Λ , where the occupation number of the negative energy modes should drop to zero. We implement this additional term by treating it as a Lagrange-multiplier method and hence we enforce the constraint $\frac{d\Psi^\dagger}{dx} \frac{d\Psi}{dx} = \kappa$ for some constant κ . According to the rules of cMPS, this translates to the condition

$$\sum_{\alpha} \text{tr} ([Q, R_{\alpha}]^{\dagger} [Q, R_{\alpha}] \rho_{ss}) = \kappa. \quad (6.53)$$

Depending on our choice of κ we see the cutoff at different momenta but we know from the above discussion that this was to be expected since different choices of κ correspond to different rescaling parameters c , which are intrinsic to the regularisation problem. We know that the drop to zero of the momentum occupation corresponds to $p = \Lambda$ independent of c and κ .

6.12 Description of our algorithm

We proceed algorithmically by first finding the steady state of the Lindbladian, which is analogous to the Lieb-Liniger case, only that we now have a sum over the species α and the new parametrization of the interaction matrices R_{α} for the fermionic case discussed above.

$$\mathcal{L}[\rho] = -i[K, \rho] + \sum_{\alpha} \left(R_{\alpha} \rho R_{\alpha}^{\dagger} - \frac{1}{2} \{ R_{\alpha}^{\dagger} R_{\alpha}, \rho \} \right) \quad (6.54)$$

We then take this and optimize the Dirac Hamiltonian expectation value under the constraint from the previous section (equation 6.53), again using the constrained optimization routine `fmincon`. This gives us the optimized matrices (Q, R_{α}) . We then use our discussion from section (4.12), which tells us that $|r\rangle = |\rho_{ss}\rangle$ and $\langle l| = \langle \mathbf{1}| = \sum_k \langle k|$. Having found the optimal (Q, R_{α}) also enables us to compute $T_{s_{\alpha}}$ simply from its definition (equation 6.13)

$$T_{s_\alpha} = \mathbf{1} \otimes Q^* + Q \otimes \mathbf{1} - \sum_{\alpha} R_{\alpha} \otimes R_{\alpha}^*, \quad (6.55)$$

which we can efficiently invert numerically to evaluate the expression gained for the number densities $n_{\alpha\beta}(p)$ [equation (6.46)], which are the central ingredient to the occupation numbers we describe in the following section.

6.13 Dirac sea

Dirac's original interpretation of the negative energy solutions to his equation was that the vacuum state should contain an infinity of particles with all negative energy states occupied. Together with the Pauli exclusion principle this guarantees that there is no instability because a particle cannot gain arbitrarily high energy by "falling" deeper into the negative part of the energy spectrum since they are already occupied. In this picture, an excitation corresponds to a hole in this Dirac sea. The modern, canonical way to fix this instability is to normal order the fields and reinterpret the non-occupied negative energy states as antiparticles, changing the role of annihilator and creator. This amounts to a shift in the energy of the vacuum, which is not an observable quantity (cosmology aside). However if we stick to the Dirac sea picture and force the cMPS method through, we should be able to observe the filling of states corresponding to $\hat{b}(p)$.

In order to do that we use the expressions for \hat{b} obtained in equation (6.37), recalling that $\langle \Psi_i^\dagger \Psi_j \rangle = n_{ij}(p)$:

$$n_{--}(p) := \langle b^\dagger(p)b(p) \rangle = \quad (6.56)$$

$$\frac{p^2}{2E_p(E_p + m)}n_{11}(p) + \frac{m + E_p}{2E_p}n_{22}(p) - \frac{ip}{2E_p}(n_{21}(p) - n_{12}(p)) \quad (6.57)$$

Ideally, we would get a step-function behaviour $n_{--} = \Theta(1 - p/\Lambda)$, meaning that all states up to the cutoff momentum are filled and states with higher momentum are empty. For the number of particles, corresponding to the positive energy solution we expect all states to be empty in the vacuum state. As shown in figure (6.1), we approximate this behaviour quite well already for $\tilde{D} = 2$. We remind the reader that $D = 4\tilde{D}$ due to the Jordan-Wigner construction (see section (6.5)). The number density for particles n_{++} and the mixing term n_{+-} are expected to be empty in the vacuum state, which is also correctly described in figure (6.2). When increasing the bond dimension to $\tilde{D} = 4$, we see (figure 6.3) that the results further improve, as the filling of states with $p < \Lambda$ is smoothed out. The filling of particles and the mixing term, which were already close to zero for $\tilde{D} = 2$, are also closer to zero as one would have expected (see figure (6.4)). This again supports our claim that cMPS is capable of correctly describing the filling of the Dirac sea. The MATLAB code corresponding to the mentioned work can be studied in the appendix to this thesis.

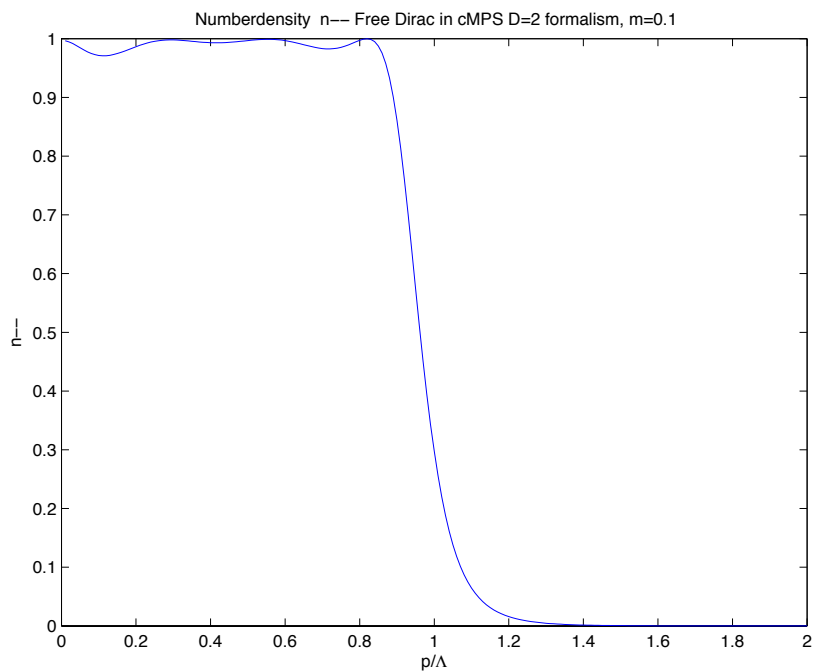


Figure 6.1: Filling the Dirac sea: $n_{--}(p/\Lambda)$ parameters: $\tilde{D} = 2$, $m = 0.1$

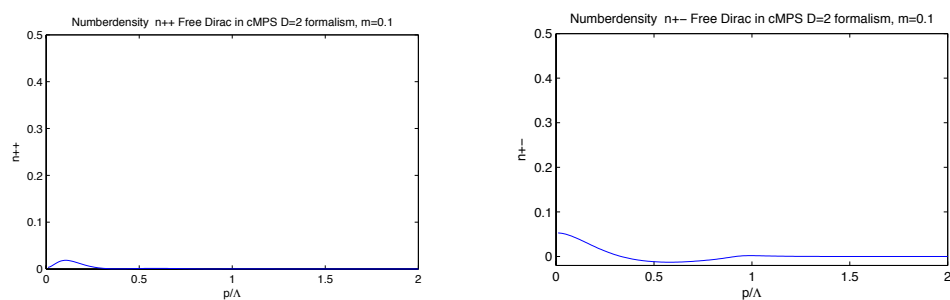


Figure 6.2: $n_{++}(p/\Lambda)$ and $n_{+-}(p/\Lambda)$ vanish, as expected. $\tilde{D} = 2$, $m = 0.1$

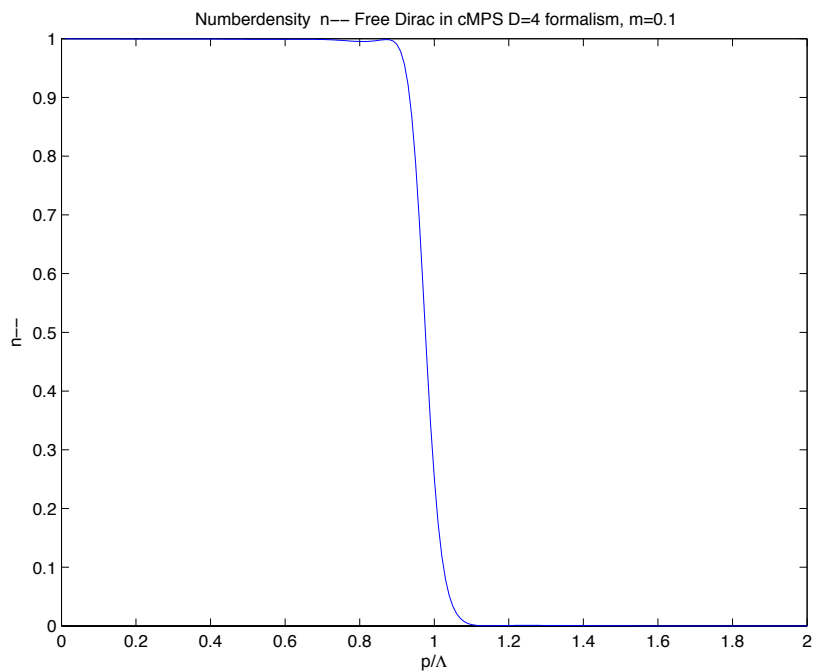


Figure 6.3: Smoothing out the filling $n_{+-}(p/\Lambda)$ by higher bond dimension. Parameters: $\tilde{D} = 4$, $m = 0.1$

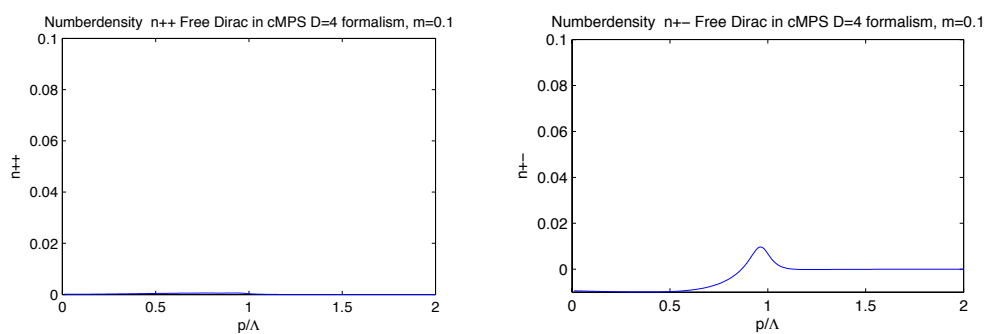


Figure 6.4: $n_{++}(p/\Lambda)$ and $n_{+-}(p/\Lambda)$ for higher bond dimension. Note that we zoom in on the y -axis. $\tilde{D} = 4$, $m = 0.1$

Chapter 7

Conclusion and Outlook

7.1 Conclusion

In this thesis we have presented the continuous matrix product state formalism. We gave a brief introduction to tensor network methods and then extended the theory to continuum field states by applying the cMPS formalism to the Lieb-Liniger and the Dirac model. For these models, we were able to implement the techniques derived from the cMPS formalism and we have convinced ourselves of the potential of these methods. A central part of this thesis was the implementation of algorithms that make use of the variational method in the cMPS formalism. We first did so for the Lieb-Liniger model where we were able to derive the correct behaviour of the ground state energy and demonstrated the convergence of the cMPS method by increasing the bond dimension. We then went on to a relativistic setting, where we analysed the free Dirac equation. We extended the cMPS formalism to fermionic systems and multiple species of particles. Furthermore the extension to a

relativistic setting was accomplished by introducing a regularisation in the form of a Lagrangian multiplier to the minimization process. This enabled us to look at the phenomenon of the filling of the Dirac sea which arises when one looks at Diracs original interpretation of negative energy solutions to his equation. We succeeded in verifying that the cMPS method is capable of reproducing this filling of the Dirac sea already with moderate bond dimension, thereby extracting sensible physics from the field system. We found a new method to find this filling by solving the dissipative dynamics on the auxiliary system and translating this to the momentum filling of states. The results of this method were found to be in accordance with the findings of [Haegeman et al. \[2010\]](#), who used imaginary time evolution.

7.2 Outlook

The cMPS formalism is a very young field of research but has already attracted interest from various perspectives. The generalisazion away from 1+1 to higher dimensional theories, most notably by the PEPS and (c)MERA formalism, is an active area of research, especially the incorporation of desirable symmetries is non-trivial and under investigation [[Jennings and Osborne](#)] et al. We expect these theories to have success comparable to the one that was enjoyed by MPS for discrete systems in the recent past. We believe, that they will be able to shed new light on the study of area laws and the classification of quantum phases. The simulation of fermonic systems, where current techniques, most notably Monte Carlo methods, break down due to the sign problem is also expected to be straightforward in these tensor net-

work methods. Due to its connection to field theory and the holographic property of cMPS and cMERA, researchers have conjectured a connection to the AdS/CFT correspondence [Nozaki et al., 2012], a major conjecture in high energy physics which is related to the holographic principle. In a general sense, variational techniques are very desirable in any quantum system since they allow us to study otherwise intractable systems to high precision.

Chapter 8

Appendix

8.1 Lieb-Liniger code

For the Lieb-Liniger model we used the following code. Line-breaks may be artificial due to limited space in this format.

```
% this is a script to find the minimal energy in the Lieb-Lininger model  
% as a function of the interaction parameter c  
  
%call the fmincon with the function energydensity and the constraint  
%particlenumber  
options = optimset('Display','Iter','Algorithm','interior-point',  
                  'MaxFunEvals', 3000);  
  
D = 2;  
x0 = rand(1,2*D*D);  
c_max = 20;  
energyarray2 = zeros(1,c_max);
```

```

for c=1:c_max
[x,fval] = fmincon(@(x)energydensity(x,c),x0,
                  [],[],[],[],[],[],@particlenumber,options);
energyarray2(c)=fval;
end
plot(energyarray2)

function [H0,R0] = extract(x)
%this defines a function to extract the matrices K (sometimes called H)
%and R from the vector x fmincon and other functions handle
%the correct parametrizations are built in here,  $K^{\dagger} = K$ 

dim = sqrt(0.5*size(x,2));

A = zeros(dim,dim);
B=zeros(dim,dim);

%fill diagonal (real
for k=1:dim
    A(k,k)=x(k);
end

%counter a
a=dim+1;

```

```
for m=1:dim
    for n=(m+1):dim
        A(m,n)=x(a)+1i*x(a+1);
        A(n,m)=x(a)-1i*x(a+1);
        a=a+2;
    end
end

B = reshape(B,1,dim*dim);

for m=1:(dim*dim)
    B(m)=x(m+dim*dim);
end

B = reshape(B,dim,dim);
HO = A;
RO = B';

function [ energy ] = energydensity(x,c)
%this is the function we minimize with fmincon

[H,R] = extract(x);

rho_ss = steadystatefinder(H,R);
Q = -0.5*R'*R -1i*H;
```

```

C = Q*R-R*Q;
C = qo(C);
R = qo(R);

energy = real(trace(rho_ss*(C'*C)+ c*rho_ss*(R*R)'+R*R));

end

function [c,ceq] = particlenumber(x)
%PARTICLENUMBER, this will be the constraint function for fmincon
c= [];
[H,R] = extract(x);
R = qo(R);
rho_ss = steadystatefinder(H,R);
ceq = real(trace(R'*R*rho_ss))-1;
end

function [ state ] = steadystatefinder(H,R)
%use Quantum optics toolbox to find steady state
% qotoolbox deals with "quantum objects" qo
H = qo(H);
R=qo(R);
L = -1i*(spre(H)-spost(H)) + spre(R)*spost(R')
      -0.5*spre(R'*R) - 0.5*spost(R'*R);
state = steady(L);
end

```

8.2 Dirac code

```

function [ energy ] = energydensity(x,m)
%this will be the function we minimize

[H,R1,R2] = extract(x);
rho_ss = steadystatefinder(H,R1,R2);
Q= -1i*H-0.5*(R1)'*R1-0.5*(R2)'*R2;
%rho_ss = full(rho_ss(:, :));

com1 = Q*R1-R1*Q;
com2 = Q*R2-R2*Q;

com1=qo(com1);
com2=qo(com2);

R1=qo(R1);
R2=qo(R2);

energy = real(trace((-com2'*R1 + com1'*R2 + m*(R1'*R1-R2'*R2))*rho_ss));
end

function [c,ceq] = constraint(x,Kappa)
%this will be our constraint function

ceq=[];

[K,R1,R2] = extract(x);

K=qo(K);
R1=qo(R1);
R2=qo(R2);

Q= -1i*K-0.5*(R1)'*R1-0.5*(R2)'*R2;

com1 = Q*R1-R1*Q;

```



```

com2 = Q*R2-R2*Q;
rho_ss = steadystatefinder(K,R1,R2);
c = real(trace(com1'*com1*rho_ss + com2'*com2*rho_ss))-Kappa;
end

function [state] = steadystatefinder(H,R1,R2)

K=qo(H);
R_1 = qo(R1);
R_2=qo(R2);
L = -1i*(spre(K)-spost(K)) + spre(R_1)*spost((R_1)')
      + spre(R_2)*spost(R_2') - 0.5*(spre(R_1'*R_1+R_2'*R_2)
      + spost(R_1'*R_1+R_2'*R_2));
state =steady(L);
end

function [H0,R0_1,R0_2] = extract(x)
%this is the extract function for the Dirac case,
%where we have built in the Jordan-Wigner construction

dim = 1/8*(sqrt(size(x,2)*4+1)-1);

A = zeros(4*dim,4*dim);

%fill diagonal (real

```

```
for k=1:4*dim
    A(k,k)=x(k);
end

%counter a
a=4*dim+1;

for m=1:4*dim
    for n=(m+1):4*dim
        A(m,n)=x(a)+1i*x(a+1);
        A(n,m)=x(a)-1i*x(a+1);
        a=a+2;
    end
end

P1 = zeros(dim,dim);
P2 = zeros(dim,dim);

for k=1:dim
    P1(k,k) = x(16*dim*dim+k)+1i*x(16*dim*dim+dim+k);
    P2(k,k) = x(16*dim*dim+2*dim+k) + 1i*x(16*dim*dim+3*dim+k);
end

%Pauli matrices
sigma_minus = [0,1;0,0];
```

```

sigma_z = [1,0;0,-1];
%Jordan-Wigner:
R_1=kron(kron(sigma_minus,eye(2)),P1);
R_2=kron(kron(sigma_z, sigma_minus), P2);
H0 = A;
R0_1 = R_1;
R0_2 = R_2;
end

%this is the script for the minimization:
D = 2;
x0 = rand(1,16*D*D+4*D);
m=0.1;

Kappa = 0.1;
options = optimset('Display','Iter','Algorithm','interior-point',
    'UseParallel', 'always','MaxIter',2000,'MaxFunEvals', 100000);

[x,fval] = fmincon(@(x)energydensity(x,m),x0,
    [], [], [], [], [], @(x)constraint(x,Kappa),options);

[K,R1,R2] = extract(x);

dim = size(K,2);
Q= -1i*K-0.5*(R1)'*R1-0.5*(R2)'*R2;

```

```

T = kron(Q,eye(dim))+kron(eye(dim),conj(Q))
      -kron(R1,conj(R1))-kron(R2,conj(R2));

R{1}=R1;
R{2}=R2;

rho_ss = steadystatefinder(K,R1,R2);
n_vs_p;

%this calculates the  $n_{\alpha\beta}(p)$  for given optimized cMPS matrices
function f = n_ab(T,R,a,b,p,rho_ss)

    RIGHTMATRIX=full(rho_ss(:, :));
    RIGHT = reshape(transpose(RIGHTMATRIX),size(RIGHTMATRIX,2)^2,1);
    id=eye(sqrt(size(RIGHT,1)));
    LEFT=id(:);
    %RIGHT=full(rho_ss(:));

    dim=sqrt(size(T,2));
    f = LEFT'*kron(eye(dim),conj(R{a}))*((-T+1i*p*eye(dim*dim))
        \kron(R{b},eye(dim)))*RIGHT
        + LEFT'*kron(R{b},eye(dim))*((-T-1i*p*eye(dim*dim))

```

```

\kron(eye(dim),conj(R{a}))) *RIGHT;

end

%this returns the momentum space occupation for n++, n-- and n+-
function f = numberdensity(p,m,T,R,rho_ss)

E_p=sqrt(p*p+m*m);

n_11=n_ab(T,R,1,1,p,rho_ss);
n_12=n_ab(T,R,1,2,p,rho_ss);
n_21=n_ab(T,R,2,1,p,rho_ss);
n_22=n_ab(T,R,2,2,p,rho_ss);

%antiparticles n--
f = p*p/(2*E_p*(m+E_p))*n_11 + (m+E_p)/(2*E_p)*n_22
    -1i*p/(2*E_p)*(n_21-n_12);

% particles n++
%f = p*p/(2*E_p*(m+E_p))*n_22 + (m+E_p)/(2*E_p)*n_11
    % +1i*p/(2*E_p)*(n_21-n_12);

%n+-
%f = p*p/(2*E_p*(m+E_p))*n_21 + (m+E_p)/(2*E_p)*n_12
    %-1i*p/(2*E_p)*(n_11-n_22);

end

```

```
numberdensityarray = zeros(1,200);

for h=1:200
    numberdensityarray(h) = numberdensity(h/100.,m,T,R,rho_ss);
end

momentum = (1:200)/100.;

plot(momentum,numberdensityarray);
title('Numberdensity Free Dirac in cMPS D=2 formalism')
xlabel('momentum')
ylabel('n--')
```

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