On the new Continuous Matrix Product Ansatz

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Abstract. The fertile new field of quantum information theory is inspiring new ways to study correlated quantum systems by providing fresh insights into the structure of their Hilbert spaces. One of the latest developments in this direction was the extension of the ubiquitous matrix-product-state constructions, epitomized by the density-matrix renormalization-group algorithm, to continuous space-time; so as to be able to describe low-dimensional field theories within a variational approach. Following the earlier success achieved for bosonic theories, we present the first implementation of a continuous matrix product state (cMPS) for spinfull non-relativistic fermions in 1D. We propose a construction of variational matrices with an efficient parametrization that respects the translational symmetry of the problem (without being overly constraining) and readily meets the regularity conditions that arise from removing the ultraviolet divergences in the kinetic energy. We tested the validity of our approach on an interacting spin-1/2 system with spin imbalance. We observe that the ansatz correctly predicts the ground-state magnetic properties for the attractive spin-1/2 Fermi gas, including a phase-oscillating pair correlation function in the partially polarized regime (the 1D correlate of the FFLO state). We shall also discuss how to generalize the cMPS ansatz to other situations.

1. Introduction

Matrix product states (MPS) are a natural class of variational states that arises in several contexts, like in the theory of 1D spin systems [1] or in the framework of the so called Density Matrix Renormalization Group (DMRG) [2, 3, 4]. (DMRG is an optimal variational ansatz for 1D lattice models [5, 6].) A coherent-state extension of the MPS ansatz to the continuum (called cMPS in the literature [7, 8, 9, 10, 11, 12, 13, 14, 15, 16]) has been introduced in the last lustrum. This new ansatz has been very successful but it is still under development. In this proceedings contribution we report on our recent progress in testing and extending cMPS in different directions.

Let us jump ahead and introduce the cMPS directly for the case of fermions. A cMPS for spin-1/2 fermions is the natural generalization of the bosonic case [7] by replacing the boson field by a fermion field and introducing a spin index ($\sigma$). Explicitly, for a system length of $L$ and periodic boundary conditions, it has the general form [10]

$$|\chi\rangle = \text{Tr}_{\text{aux}}[P e^{i\int_0^L dx [Q(x)\hat{I} + \sum_{\sigma} R_{\sigma}(x) \hat{\psi}_\sigma^\dagger(x)]}] |\Omega\rangle,$$

where $Q(x)$ and $R_{\sigma}(x)$ are $\mathbb{C}^{D\times D}$ matrices that act on a $D$-dimensional auxiliary space and $D$ is called the bond dimension. $\hat{I}$ is the identity operator on the Fock space of the bosons ($\hat{\phi}^\dagger$) or the fermions ($\hat{\psi}_\sigma^\dagger$), $\text{Tr}_{\text{aux}}$ indicates the trace over the auxiliary space, $P$ is a path-ordering.
Figure 1. Energy density per particle of the repulsive Lieb-Liniger model as a function of interaction strength ($g$). The results are given for bond dimensions $D = 2, 4, 6, 8$. The solid line is the exact result as obtained using Bethe’s Ansatz.

prescription for the exponential function of Fock-space operators, and $|\Omega\rangle$ is the Fock-space vacuum state.

2. Test Cases

In order to test the performance of the cMPS ansatz and demonstrate its virtues and limitations, we apply it in what follows to three paradigmatic interacting systems, the first two being bosonic and fermionic gases in 1D and the third one a 1D-lattice model of spins. All three models admit exact analytic solutions against which we can compare the cMPS variational results.

2.1. Bosons: the Lieb-Liniger model

The so called Lieb-Liniger model [17] consists of bosons interacting via a repulsive contact potential:

$$H_{\text{LL}} = \int_0^L dx \left( \partial_x \hat{\phi}^\dagger \partial_x \hat{\phi} + 2\Delta (\hat{\phi}^\dagger \hat{\phi}^\dagger \hat{\phi} \hat{\phi}) \right), \tag{2}$$

where $\Delta = g/2$ is positive for repulsive interactions.

The results of applying the cMPS variational ansatz to this model were first presented in the same work that introduced the cMPS as an ansatz idea [7]. We show in Fig. 1 how we reproduce those results using our own variational minimization scheme that we will use again below to apply it to other cases. As the bond dimension grows, the cMPS variational results quickly improve and approach the exact result that we obtained via Bethe’s Ansatz.
Figure 2. Free energy densities along a circular trajectory centered at the triple point of the attractive Gaudin-Yang model (see Fig. 2 of Ref. [16]). From Ω to Ψ the external magnetic field increases but, due to the competition with pairing due to the interaction, the system remains in a homogeneous quasi-superfluid state. From Ψ to Y the field is even larger and the system remains in a quasi-superfluid state but develops a pair-density-wave order (without breaking translational invariance). Finally, form Y to X the applied field is beyond a density-dependent threshold and the ground state is fully polarized (and thus non-interacting and well described by a mean-field calculation). The results are given for three different bond dimensions, $D = 4, 8, 16$. The solid line is the exact result as obtained using Bethe’s Ansatz and the dashed line is the result from a Bogoliubov-deGennes calculation.

2.2. Fermions: the Gaudin-Yang model

The same as for DMRG, which was generalized to fermions (including the calculation of full dynamic correlators [18]) only several years after its initial introduction, the cMPS ansatz was extended to fermions (with full treatment of the interactions) only earlier this year [16]. This was done in the context of interacting 1D gases with spin imbalance that have been recently realized in cold-atom systems [19] and motivated a large amount of work using other techniques [20, 21, 22, 23, 24, 25, 26, 27]. It thus constitutes a highly non-trivial but well understood test case; with the added excitement of being the least controversial concrete realization of the so called FFLO superfluid state [28, 29] (albeit in a one-dimensional sense).

The so called Gaudin-Yang Hamiltonian [30, 31] is the natural generalization of the Lieb-Liniger case to fermions. In this model, spin-1/2 fermions interact via a contact potential and one writes

$$H_{GY} = \int_{0}^{L} dx \sum_{\sigma = \uparrow, \downarrow} \left( \partial_x \hat{\psi}_\sigma^{\dagger} \partial_x \hat{\psi}_\sigma - 2\Delta \hat{\psi}_\sigma^{\dagger} \hat{\psi}_\sigma \hat{\psi}_\sigma \hat{\psi}_\sigma \right),$$

where $\bar{\sigma}$ denotes the spin conjugate to $\sigma$, and the interaction strength $\Delta$ is negative or positive for repulsive or attractive interactions, respectively.
Figure 3. Densities of the majority (blue) and minority (red) fermions, and their difference (green), along the same trajectory as in the previous figure (see Fig. 2). The same three different bond dimensions as before are again compared to the exact results (solid lines).

Applying the fermionic version of the cMPS ansatz we obtained the results shown in Figs. 2 and 3 for the free energy and particle densities, respectively.

Inspired by comparisons with the wave function of Bethe's Ansatz [16], we dropped the spatial dependence of $Q(x) = Q$ and introduced a phase modulation on $R_\sigma(x) = R_\sigma e^{iq_\sigma x}$. Now $Q$ and $R_\sigma$ are complex-valued $D \times D$ matrices independent of position, and the $q_\sigma$’s are additional real-valued variational parameters.

Regularity of the kinetic-energy density requires imposing the additional conditions:

$$\{R_{\uparrow}, R_{\downarrow}\} = 0 \quad \text{and} \quad R_\sigma^2 = 0. \quad (4)$$

which we showed how to implement with great generality in Ref. [16].

In here we introduced an additional overall similarity transformation to the definition of the $R_\sigma$ matrices, which provides additional freedom to impose the cMPS-gauge condition $Q = -\frac{1}{2}(R_{\uparrow}^R R_{\downarrow} + R_{\downarrow}^R R_{\uparrow}) - iH$, where $H$ is an arbitrary Hermitian matrix. This additional freedom gives improved free-energy estimates for lower bond dimensions ($D = 4, 8$) and some improvements also for the densities (cf. Ref. [16]), although the determination of the location of some of the phase boundaries is still as delicate as before.

The results are in general good agreement with the exact solution, but cMPS allow us to go further and compute quantities like two- and four-point correlators that are notoriously difficult to obtain from Bethe’s Ansatz (this has been shown already in Ref. [16], where we demonstrated the appearance of FFLO-type pair-pair correlations in the relevant part of zero-temperature phase diagram).

The good agreement in the strictly 1D case makes cMPS very promising for extensions to quasi-1D scenarios like the tube arrays that are actually used in the experiments. Other methods have already shown that there is a wide and rich spectrum of physical behaviors to be expected in such systems [32, 33, 34].
Figure 4. Energy of the transverse-field Ising chain for bond dimension $D = 4$ shown as a function of $g = \hbar/J$. The solid line corresponds to the exact analytic solution of the model.

2.3. Spins: the quantum Ising model

During our presentation, we showed also preliminary results of applying the cMPS ansatz to the quantum Ising model (also known in the literature as the transverse-field Ising model). The Hamiltonian of the system is given by

$$H_{\text{qI}} = -J \sum_{\langle i,i' \rangle} \sigma_i^x \sigma_{i'}^x - h \sum_i \sigma_i^z,$$

(5)

where the angular brackets mean summation over ‘near-neighbor pairs’. $J > 0$ corresponds to the ferromagnetic case which we will be studying (many results would be similar for the antiferromagnetic case with $J < 0$). Here $\sigma_i^{x,z}$ are Pauli matrices and the system is considered in a ring or with periodic boundary conditions (i.e., lattice sites $i = 1$ and $i = L$ are neighbors).

There are a number of ways of applying cMPS to this system, the most direct for us being by mapping first to fermions via a Jordan-Wigner transformation and taking the lattice spacing as if it were the lattice regularization of cMPS. In this way the cMPS ansatz connects naturally to the continuum limit of the model (typically used for analytic studies of its quantum-critical properties).

Results for the energy and the magnetization along the $x$-axis are shown on Figs. 4 and 5, respectively, and they are compared to the exact solution of the model [35].

While the agreement in terms of energy is uniformly good, the magnetization proves to be a more difficult quantity. The magnetization along the field axis is obtained by direct calculation, with an agreement that is as good as that for the energy (and indeed can also be obtained from the numerical derivative of the result in Fig. 4). But, contrarily, the transverse magnetization is only in good agreement for sub-critical transverse fields. For larger fields cMPS incorrectly gives a non-zero magnetization, while an indirect argument based on the exact solution predicts a sharp transition to a zero value. This is therefore a very sharp transition that provides a stringent test case for cMPS and will be very useful in order to understand it and developing it further (which is work in progress).
Figure 5. Magnetization along the easy magnetic axis of the exchange interaction, and thus transverse to the field, as a function of $g = h/J$ (cf. Fig. 4). The solid line corresponds to the indirect analytic solution.

3. Conclusions
To summarize, we have demonstrated on three concrete examples the validity and accuracy of cMPS by comparing with available exact solutions. In general, the variational approach can provide additional physical information that is not always easy to extract from the analytic solutions and provides different physical insights. Moreover, as the cMPS ansatz is generic and not restricted to integrable Hamiltonians, we envisage that our work would open the doors to solving outstanding 1D problems and shed light on our understanding of interacting theories of bosons, fermions, spins, or their mixtures.

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