Extended abstract of Ref. [1]

Matrix product operators and states: NP-hardness and undecidability

Martin Kliesch[1], David Gross[2], and Jens Eisert[1]

[1]Freie Universität Berlin, 14195 Berlin, Germany

[2]Universität Freiburg, 79104 Freiburg, Germany

Tensor network states constitute an important variational set of quantum states for numerical studies of strongly correlated systems in condensed-matter physics, as well as in mathematical physics. This is specifically true for finitely correlated states or matrix-product operators, designed to capture mixed states of one-dimensional quantum systems. It is a well-known open problem to find an efficient algorithm that decides whether a given matrix-product operator actually represents a physical state that, in particular, has no negative eigenvalues. We address and answer this question by showing that the problem is provably undecidable in the thermodynamic limit and that the bounded version of the problem is NP-hard in the system size. We discuss the profound consequences for the description of quantum many-body systems using tensor networks. This work shows how ideas of computer science can help to address key problems of quantum many-body physics beyond questions of Hamiltonian complexity.

Keywords: Tensor network states, matrix product operator (MPO), finitely correlated state (FCS), NP-hardness, undecidability, intersection of computer science and many-body physics

Computational quantum many-body physics is marred by the fact that standard computational descriptions of states require exponentially many parameters. Fortunately, for many physically relevant problems, one does not need to consider all those parameters to capture natural properties extremely accurately. One of the pillars on which computational many-body approaches rest is the framework of tensor network methods. Here, the relevant degrees of freedom are parameterized by very few numbers which are organized in terms of tensor networks that are contracted in order to compute expectation values [2–9]. Notably, the *density-matrix renormalization group approach*, the most successful method to numerically determine ground state properties of strongly correlated one-dimensional models, can be cast into such a form [2, 3]. In this language, the problem of minimizing the energy can be phrased as a variational principle over *matrix product* (or *purely generated C^*-finitely correlated*) *states* [10]. The natural analogue that also encompasses mixed quantum states are *matrix product operators* (MPOs). Again, they feature strongly in numerical algorithms [11, 12], for example when investigating stationary states of local Liouvillians modelling open quantum systems [13, 14] or Gibbs states [15, 16]. However, general MPOs are not guaranteed to represent physical states, which is the source of considerable conceptual and computational difficulties. It would thus be highly desirable to design an efficient algorithm capable of checking whether a given matrix product representation defines a positive operator (see Figure 1). To decide if such an efficient "local test for positivity" exists is a fundamental problem in the field, implicit already in its early formulations [10].

Here, we address and answer this question: Determining whether an MPO defines a physical state in the thermodynamic limit is a provably *undecidable problem*. We also show that the bounded version of the problem is NP-hard in the number of tensors, burying hopes that one could find an efficient algorithm testing for positivity exactly. This is proven for quantum spin chains with local dimension $d = 2$ by a polynomial reduction from the *Post correspondence problem* and a bounded variant thereof.

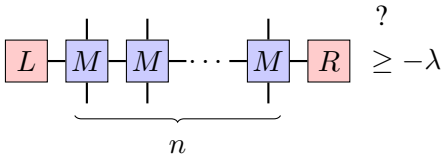

Figure 1: An MPO as a tensor network. The problem is to determine whether or not this defines a positive operator.

To give a practical example: One can approximate stationary states of local Liouvillians by iteratively applying the Liouvillian to a state described as an MPO and subsequently truncating the tensors. To avoid inconsistent results, one has to check whether the truncation step has caused the state to become "too unphysical" in that it has created eigenvalues that are more negative than some chosen tolerance threshold. This we prove to be infeasible. The practical implications of our work are as follows: One hand they motivate the quest for finding specific feasible instances that might exist. This quest reminds of the task of finding efficient contractions of two-dimensional planar tensor networks, even though this task has been identified to be #P-complete [17]. On the other, it shows that one should direct one's efforts towards finding approximate solutions. The insight presented here adds a natural many-body problem to the list of quantum mechanical questions that have recently been identified not only as computationally hard, but as outright undecidable [18–21]. We also point out connections to the theory of hidden Markov models.

Results

In the statements of the various problems below, MPO-tensors are specified by rational numbers. These have finite descriptions and can thus serve as inputs to algorithms. Allowing for more general numbers (e.g. algebraic numbers) would make the problem only harder. Our results are stated for MPOs of the following translation invariant form:

Definition 1 (Matrix product operator (MPO))**.** *An instance of* MPO-tensors *is given by a tensor* $M = \left(M_{i,j}^{(\alpha,\beta)}\right)_{\alpha,\beta\in[d],\, i,j\in[D]} \in \mathbb{Q}^{d\times d\times D\times D}$ *and vectors* $|L\rangle, |R\rangle \in \mathbb{Q}^D$*. The dimension* d *is called* physical dimension *and* D (MPO)-bond dimension*. The generated translation invariant* MPO *for* system size n *is*

$$\rho(L, M, R, n) := \sum_{j\in[D]^{n+1}} L_{j_1} M_{j_1,j_2} \otimes \cdots \otimes M_{j_n,j_{n+1}} R_{j_{n+1}}.$$

In the precise statement of the problem, we allow for a threshold λ which bounds the "degree of negativity" that is deemed acceptable. (We call positive semi-definite operators just *positive*.)

Problem 2 (Bounded MPO threshold problem (BTP))**.**
Instance: *MPO-tensors* M*,* $|L\rangle$*, and* $|R\rangle$*, threshold* $\lambda \in \mathbb{Q}$*, and system size* n*.*
Question: *Is the MPO* $\rho(L, M, R, n) + \lambda\mathbb{1}$ *positive?*

Problem 3 (MPO threshold problem (TP))**.** *The* TP *is defined in the same way as its bounded version above except that there is no restriction on the system size and the question is: Is there an* $n \in \mathbb{Z}^+$ *such that* $\rho(L, M, R, n) + \lambda\mathbb{1}$ *is* not *positive?*

We obtain the following results these problems to be not tractable on classical computers.

Theorem 4 (NP-hardness of the bounded MPO threshold problem)**.** *For any* $\lambda \in \mathbb{Q}$ *and physical dimension* $d \geq 2$*, the* BTP *is* NP*-hard.*

Theorem 5 (Undecidability of the MPO threshold problem)**.** *For each threshold $\lambda \in \mathbb{Q}$ the* TP *is undecidable. In particular, this holds for the case where the physical dimension is $d = 2$, the bond dimension is $D = 42$, and the matrices $M_{i,j}$ are diagonal for all $i, j = 1, \ldots, D$.*

We end by sketching two corollaries of these results. In Ref. [30] local purifications of positive MPOs in terms of matrix product states are investigated and it is shown that the arising MPS-bond dimension can in general not be bounded independently of the system size. This suggests that such purifying MPS would require high bond dimensions when used instead of MPOs in numerical simulations. The authors go on to describe two explicit algorithms that construct purifying MPS given an MPO representation. These algorithms are not in general efficient, and the natural question arises whether an efficient algorithm might be identified in the future. As a consequence of our Theorem 4 we obtain:

Corollary 6 (Purifying matrix-product states)**.** *There is no polynomial-time algorithm that can convert an MPO representation into a purifying MPS.*

Along different lines, there has been a recent surge of interest in using efficient many-body descriptions for the purpose of quantum state tomography of large systems [31–33]. The most explicit work makes use of MPO rather than purifying MPS [32] and provides an efficient algorithm. We can now show that a similar result for purifying MPS is not possible:

Corollary 7 (Tomography)**.** *There is no polynomial-time algorithm for reconstructing a state with an efficient purifying MPS description from local physical measurements performed on it.*

Conclusions and outlook

Finally, we comment on ways to efficiently detect negativity locally by calculating expectation values with respect to matrix product states (MPS) of small bond dimension. In the BTP one is asked to *exactly* delineate the MPOs with smallest eigenvalues above $-\lambda$ from those with smallest eigenvalues below $-\lambda$. In practice, it would be acceptable if an algorithm reliably recognizes whether a state ρ is either sufficiently positive, i.e., $\rho \geq -\lambda$, or violates a threshold by at least $\epsilon \geq 0$, i.e., $\rho \ngeq -(\lambda + \epsilon)$. Such an approximate version is allowed to give unspecified results on the narrow band between the two cases. In order to make this precise, we state the BTP as a *weak membership problem*. The MPO provided in the proof of Theorem 4 has a trace that is exponentially bounded from above. Hence, as a corollary, one obtains that the BTP remains NP-hard as a weak membership problem if ϵ is exponentially small in n. This statement remains true for algebraic and not necessarily rational inputs. Weak membership formulations seem to be natural for a variety of problems in quantum information. For instance, NP-hardness of testing separability of quantum states as a weak membership problem was established first [34] for an exponentially small "error" ϵ and, much later [35], for a polynomially small ϵ, in fact, using key methods of the previous approach [34]. Hence, our work is an invitation to explore whether the BTP as a weak membership problem is also NP-hard for only polynomially bounded ϵ or, instead, to actually find an algorithm that efficiently solves that problem. Another important question is whether there are physically relevant instances for which positivity is efficiently decidable and how this can be exploited best in numerical algorithms.

This work shows that ideas of computer science can help to make progress on questions in the theory of open and closed quantum many-body systems, beyond questions that are usually considered in the context of Hamiltonian complexity. It also invites a plethora of future research directions. It would be a significant step forward, one the one hand, to find instances and approximations where (near-)positivity can be guaranteed. On the other, this can be seen as the start of the program of identifying those problems in the context of tensor network states that are not decidable algorithmically.

References

[1] M. Kliesch, D. Gross, and J. Eisert, in print in Phys. Rev. Lett., arXiv:1404.4466 (2014).
[2] S. Rommer and S. Ostlund, Phys. Rev. B **55**, 2164 (1997).
[3] U. Schollwoeck, Ann. Phys. **326**, 96 (2011).
[4] F. Verstraete, J. I. Cirac, and V. Murg, Adv. Phys. **57**, 143 (2008).
[5] N. Schuch, arXiv:1306.5551.
[6] R. Orus, arXiv:1306.2164.
[7] J. Eisert, Modeling and Simulation **3**, 520 (2013).
[8] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quant. Inf. Comput. **7**, 401 (2007).
[9] J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys. **82**, 277 (2010).
[10] M. Fannes, B. Nachtergaele, and R. F. Werner, Comm. Math. Phys. **144**, 429 (1992).
[11] F. Verstraete, J. J. Garcia-Ripoll, and J. I. Cirac, Phys. Rev. Lett. **93**, 207204 (2004); arXiv:cond-mat/0406426.
[12] M. Zwolak and G. Vidal, Phys. Rev. Lett. **93**, 207205 (2004); arXiv:cond-mat/0406440.
[13] M. C. Banuls, *Tensor network techniques for the study of dissipative dynamics*, talk held in Stellenbosch, April 19 (2013).
[14] Z. Cai and T. Barthel, Phys. Rev. Lett. **111**, 150403 (2013).
[15] T. Barthel, U. Schollwöck, and S. R. White, Phys. Rev. B **79**, 245101 (2009).
[16] E. M. Stoudenmire and S. R. White, New J. Phys. **12**, 055026 (2010).
[17] N. Schuch, M. M. Wolf, F. Verstraete, J. I. Cirac, Phys. Rev. Lett. **98**, 140506 (2007).
[18] J. Eisert, M. P. Muller, and C. Gogolin, Phys. Rev. Lett. **108**, 260501 (2012).
[19] M. M. Wolf, T. S. Cubitt, and D. Perez-Garcia, arXiv:1111.5425.
[20] J. Morton and J. Biamonte, Phys. Rev. A **86**, 030301(R) (2012).
[21] T. S. Cubitt, D. Perez-Garcia, and M. M. Wolf, *Undecidability of the spectral gap problem*, talk given at XVII Conference on Quantum Information Processing, Barcelona, Feb. 6 (2014).
[22] M. Vidyasagar, Math. Control Signals Syst. **23**, 1 (2011).
[23] M. Fox and H. Rubin, Ann. Math. Stat. **39**, 938 (1968).
[24] S. W. Dharmadhikari and M. G. Nadkarni, Ann. Math. Stat. **41**, 207 (1970).
[25] R. V. Erickson, Ann. Math. Stat. **41** 843 (1970).
[26] G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004).
[27] I. V. Oseledets, SIAM J. Sci. Comput. **33**, 2295 (2011); I. V. Oseledets and E. E. Tyrtyshnikov, SIAM J. Sci. Comput. **31**, 3744 (2009).
[28] M. Guta and J. Kiukas, arXiv:1402.3535.
[29] O. E. Barndorff-Nielsen, U. Franz, R. Gohm, B. Kümmerer, and S. Thorbjørnsen, *Quantum independent increment processes II* (Springer, Heidelberg, 2006).
[30] G. De las Cuevas, N. Schuch, D. Pérez-García, and J. I. Cirac, New J. Phys. **15**, 123021 (2013).
[31] M. Cramer, M. B. Plenio, S. T. Flammia, D. Gross, S. D. Bartlett, R. Somma, O. Landon-Cardinal, Y.-K. Liu, and D. Poulin, Nat. Commun. **1**, 149 (2010).
[32] T. Baumgratz, D. Gross, M. Cramer, and M. B. Plenio, Phys. Rev. Lett. **111**, 020401 (2013).
[33] T. Baumgratz, A. Nüßeler, M. Cramer, and M. B. Plenio, New J. Phys. **15**, 125004 (2013).
[34] L. Gurvits, Proc. 35th ACM Symp. Th. Comp. **10** (2003).
[35] S. Gharibian, Quant. Inf. Comp. **10**, 343 (2010).
[36] E. Post, Bull. Amer. Math. Soc. **52**, 264 (1946).
[37] "Unary notation" effectively means that the problem size of the input n equals n.
[38] Y. Matiyasevicha and G. Sénizergues, Theoret. Comput. Sci. **330**, 145 (2005).
[39] M. Sipser, "*Introduction to the Theory of Computation*", 2nd ed. (Thomson Course Technology, Boston, 2005).
[40] M. Hirvensalo, LNCS **4362**, 309 (2007).
[41] V. D. Blondel and J. N. Tsitsiklis, Inform. Process. Lett. **63**, 283 (1997).
[42] J. E. Hopcroft, R. Motwani, J. D. Ullman, *Introduction to automata theory, languages, and computation* (Pearson Addison Wesley, 2007).
[43] T. J. Osborne, arXiv:1106.5875.
[44] D. Aharonov, I. Arad, Z. Landau, and U. Vazirani, arXiv:1011.3445.
[45] S. A. Vavasis, SIAM J. Optim. **20**, 1364 (2009).
[46] D. D. Lee and H. S. Seung, Nature **401**, 788 (1999).
[47] D. D. Lee and H. S. Seung, Adv. Neural Inform. Process. Systems **13**, 556 (2000).
[48] S. Fiorini, S. Massar, S. Pokutta, H. R. Tiwary, and R. de Wolf, Proc. ACM STOC **44**, 95 (2012); arXiv:1111.0837.
[49] M. Yannakakis, Proc. ACM STOC **20**, 223 (1988).
[50] J. Gouveia, P. A. Parrilo, and R. Thomas, Math. Oper. Res. **38**, 248 (2013); arXiv:1111.3164.
[51] R. de Wolf, SIAM J. Comput. **32**, 681 (2003).
[52] C. Stark, arXiv:1210:1105.
[53] C. D. Aliprantis and R. Tourky, *Cones and Duality* (American Mathematical Society, Providence, 2007).
[54] S. Fiorini, S. Massar, M. K. Patra, and H. Raj Tiwary, arXiv:1310.4125.
[55] S. W. Dharmadhikari, Ann. Math. Statist. **34**, 705 (1963).
[56] J. Barrett, Phys. Rev. A **75**, 032304 (2007).
[57] H. Barnum, J. Barrett, M. Leifer, and A. Wilce, quant-ph/0611295.
[58] A. S. Holevo, *Probabilistic and Statistical Aspects of Quantum Theory* (North Holland, Amsterdam, 1982).
[59] D. Gross, M. P. Mueller, R. Colbeck, and O. C. O. Dahlsten, Phys. Rev. Lett. **104**, 080402 (2010).