

A polynomial-time algorithm for the ground state of 1D gapped local Hamiltonians

Zeph Landau, Umesh Vazirani, Thomas Vidick

Computing ground states of local Hamiltonians is a fundamental problem in condensed matter physics and is the quantum analog of constraint satisfaction problems. The problem is known to be QMA-complete, even for one-dimensional Hamiltonians [1]. This means that we do not even expect that there is a sub-exponential size classical description of the ground state that allows efficient computation of local observables such as the energy. In sharp contrast, the widely used heuristic density matrix renormalization group (DMRG) algorithm invented two decades ago [5] has been remarkably successful in practice on one-dimensional problems. The situation is reminiscent of the unexplained success of the simplex algorithm before the advent of ellipsoid and interior-point methods. Is there a principled explanation for this, in the form of a large class of one-dimensional Hamiltonians whose ground states can be provably efficiently approximated? Here we give such an algorithm for gapped one-dimensional Hamiltonians: our algorithm outputs a δ -approximation to the ground state, expressed as a matrix product state (MPS) of polynomial bond dimension. The running time of the algorithm is polynomial in the number of qudits n and the approximation quality δ .

Formally, consider the Hamiltonian $H = \sum_{i=1}^{n-1} H_i$ acting on n d -dimensional qudits, where H_i acts on qudits $\{i, i+1\}$ with $0 \leq H_i \leq 1$. We shall assume there is a constant gap $\varepsilon := \varepsilon_1 - \varepsilon_0$ between the energy ε_0 of the ground state (lowest energy eigenstate) $|\Gamma\rangle$ and the energy ε_1 of the first excited state. Our goal is to efficiently find a succinct description (an MPS) of an approximation to $|\Gamma\rangle$.

Of course, it is not a priori clear that such a succinct description even exists for ground states of gapped 1D systems: that they do was a consequence of Hastings' seminal proof of an area law for gapped 1D systems [2] (thus showing that the problem of finding such an MPS approximation is in NP). Unfortunately, folklore placed strong doubts on the possibility of actually designing a polynomial time algorithm for finding such a MPS approximation. This viewpoint was reinforced by results from [3] showing that a closely related problem is as hard as factoring. The recent sub-exponential algorithm [4], resulting from combining new structural results with a dynamic programming-based algorithm [5, 3], called the folklore into question, and was the starting point of our investigation.

In general, finding a minimum energy state can be expressed as a convex optimization problem: $\min \text{tr}(H\sigma)$ subject to $\text{tr}(\sigma) = 1$, $\sigma \geq 0$, where σ is a n -qubit density matrix describing the state. The problem is that the dimension of the space on which σ lives is exponentially large. Moreover, the 1D constraint, which in the classical case allows the problem to be decomposed into constant number of "boundary problems" to the left and right of any qubit, does not appear to help in the quantum case, since a similar decomposition involves exponentially (or sub-exponentially when taking the area law into account) many boundary problems. The design of the algorithm requires a number of ideas to bypass these barriers. Here we highlight two key innovations.

The first is our measure of progress as we step along in our algorithm. At the i th step of the algorithm, we find a subspace S_i of the Hilbert space of the leftmost i qubits with the guarantee that a good approximation

for the ground state $|\Gamma\rangle$ can be found within $S_i \otimes R$ where R is the Hilbert space of the rightmost $n - i$ particles. Such a subspace S_i is termed a *viable set*. Our algorithm is designed so that at each step it finds a viable set whose dimension is bounded by $\text{poly}(n)$.

Keeping the dimension at such a low level (an exponentially small fraction of the complete Hilbert space) requires us to make very coarse approximations when extending the viable set from left to right. Our second innovation consists in the construction of an operator whose application improves the approximation quality at any given step, while not blowing up the description size of the vectors in the viable set. Such an operator is called an AGSP [6]. It can be understood as an efficiently applicable “guide” through the exponentially large Hilbert space, improving any close enough approximation to the ground state in a much more efficient manner than natural imaginary-time evolution (i.e. application of e^{-Ht}). It is this ability to improve the approximation guarantee that allows the number of boundary problems to be reduced from exponential to polynomial. Our construction of the AGSP is particularly simple and relies on matrix valued Chernoff bounds for its correctness. This AGSP may be of independent interest beyond the scope of this algorithm, such as quantum algorithms based on efficient Hamiltonian simulation.

The algorithmic ideas introduced in this paper may prove helpful in tackling 2D problems, the holy grail in the field. Specifically, for 2D problems, the MPS formalism has been fruitfully generalized to PEPS [7], though these do not present any obvious way of efficiently computing local observables. A potential solution is that local observables in the 2D situation can naturally be mapped to a 1D problem by applying the transfer matrix formalism to represent a 2D network as the result of successive compositions, along the vertical axis, of a horizontal 1D matrix-product operator [8].

References

- [1] D. Aharonov, D. Gottesman, S. Irani, and J. Kempe, “The power of quantum systems on a line,” *Communications in Mathematical Physics*, vol. 287, no. 1, pp. 41–65, 2009.
- [2] M. B. Hastings, “An area law for one-dimensional quantum systems,” *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2007, no. 08, p. P08024, 2007.
- [3] N. Schuch and J. I. Cirac, “Matrix product state and mean-field solutions for one-dimensional systems can be found efficiently,” *Phys. Rev. A*, vol. 82, p. 012314, 2010.
- [4] I. Arad, A. Kitaev, Z. Landau, and U. Vazirani, “An area law and sub-exponential algorithm for 1D systems,” in *Proceedings of the 4th Innovations in Theoretical Computer Science (ITCS)*, 2013.
- [5] D. Aharonov, I. Arad, and S. Irani, “Efficient algorithm for approximating one-dimensional ground states,” *Phys. Rev. A*, vol. 82, p. 012315, 2010.
- [6] I. Arad, Z. Landau, and U. Vazirani, “Improved one-dimensional area law for frustration-free systems,” *Phys. Rev. B*, vol. 85, p. 195145, 2012.
- [7] F. Verstraete, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, “Criticality, the area law, and the computational power of projected entangled pair states,” *Phys. Rev. Lett.*, vol. 96, p. 220601, Jun 2006.
- [8] J. I. Cirac, D. Poilblanc, N. Schuch, and F. Verstraete, “Entanglement spectrum and boundary theories with projected entangled-pair states,” *Phys. Rev. B*, vol. 83, p. 245134, Jun 2011.