Quantum Many-body Bootstrap

Xizhi Han
Department of Physics, Stanford University, Stanford, CA 94305-4060, USA

A numerical bootstrap method is proposed to provide rigorous and nontrivial bounds in general quantum many-body systems with locality. In particular, lower bounds on ground state energies of local lattice systems are obtained by imposing positivity constraints on certain operator expectation values. Complemented with variational upper bounds, ground state observables are constrained to be within a narrow range. The method is demonstrated with the Hubbard model in one and two dimensions, and bounds on ground state double occupancy and magnetization are discussed.

Introduction.— Understanding ground states of interacting many-body systems remains a central challenge in quantum physics. In general, the problem is intrinsically difficult [1] and advances are often made with the aid of symmetries, approximations and numerics. Conformal symmetry and positivity have proved to be powerful in constraining correlators of quantum fields, via the conformal bootstrap [2]. In this work the positivity constraints are applied to lattice systems without conformal invariance. Similar methods for solving many-body quantum mechanics with matrix degrees of freedom are proposed in [3, 4].

The bootstrap approach in this work is also a generalization of the established variational reduced density matrix theory [5, 6] to infinite lattices. In that method, the energy is minimized while the positivity constraints are imposed for few-body reduced density matrices, yielding lower bounds for ground state energies. Previous works (e.g., [7–10]) mostly deal with all two-body reduced density matrices, and hence the computational complexity is polynomial in system size. To better utilize geometric locality of the problem, I instead consider spatially local operators only. This allows me to systematically probe more-body operators and bootstrap directly in the thermodynamic limit.

The method is demonstrated with the repulsive Hubbard model in one and two dimensions [11]. In one dimension, exact solutions are available for comparison [12]. Significant numerical progress has been made in two-dimensional cases [13–15]. Lower bounds on ground state energies are obtained by bootstrap and are consistent with the established results (see Table I and II). The algorithm is more efficient than evaluating the Anderson model [16–18].

The lower bounds are complementary to the variational upper bounds given by existing numerical approaches [13]. Often the ground state energy and observables are then pinned down in a narrow range. Such rigorous constraints on ground state observables are not generally accessible to variational methods. As an example, nontrivial bounds on double occupancy and antiferromagnetic ordering in the two-dimensional Hubbard model ground states are obtained in Table III and IV.

Method.— The many-body bootstrap is based on symmetry and unitarity in quantum mechanics. Specifically, denote \( \langle O \rangle = \text{tr}(\rho O) \), where \( \rho \) is some density matrix, then for any operator \( O \),

\[
⟨I⟩ = 1, \quad ⟨O⟩ = ⟨O⟩^*, \quad ⟨O^†O⟩ ≥ 0. \tag{1}
\]

Furthermore, \( ⟨U^{-1}OU⟩ \) = \( ⟨O⟩ \) if \( U \) is a symmetry of the state \( \rho \), i.e., \( UρU^{-1} = ρ \). If the symmetry is generated by a conserved charge \( C \), also \( ⟨[C,O]⟩ = 0 \). Thermal states and energy eigenstates are time translation invariant, so \( ⟨[H,O]⟩ = 0 \) with \( H \) the Hamiltonian and \( O \) an arbitrary operator.

Lower bounds on ground state energies are obtained by minimizing \( ⟨H⟩ \) subject to the constraints (1). More precisely, the minimization is done over the following set \( A \) of linear functionals \( F \) of operators:

\[
A = \{ F : F[I] = 1, \quad F[O^†] = F[O]^*, \quad F[[O_\alpha,O]] = 0, \quad F[U_\alpha^{-1}OU_\alpha] = F[O], \quad \forall O \in C_1, \quad F[O^†O] ≥ 0, \quad \forall O \in C_2 \}. \tag{2}
\]

Minimization over this subset of functionals is equivalent to searching for operator expectation values \( ⟨O⟩ = F[O] \) with the constraints (1). Here \( C_\alpha \) and \( U_\alpha \) are generators of the continuous and discrete symmetries to be imposed on the state. In practice the constraints (1) can only be imposed for a subset of operators \( C_1 \) and \( C_2 \). Choice of \( C_1 \) and \( C_2 \) affects computational efficiency of the algorithm, and an empirical choice in fermionic lattice models will be discussed shortly.

The true ground state energy \( E_0 \) is bounded below by the minimal value from \( F \in A \):

\[
E_0 ≥ \min_{F \in A} F[H] =: E_{lb}, \tag{3}
\]

because the functional \( F[O] = \text{tr}(\rho_0 O) \) is always in \( A \) for a ground state \( ρ_0 \) of \( H \) that also commutes with all the charges \( C_\alpha \) and \( U_\alpha \). The minimization in (3) can be solved efficiently and accurately by semidefinite programming (e.g., with [19, 20]).

The equality in (3) is reached when \( C_1 \) and \( C_2 \) are the full set of operators. Hence it is expected that the lower
bound (3) becomes tight as the number of constraints is increased. Indeed, any linear functional $F$ can be written as $F[O] = \text{tr}(FO)$ for some operator $F$. And $F$ is a density matrix (positive with unit trace) if and only if (1) holds for any $O$. Thus by the variational principle $F[H] = \text{tr}(FH)$ is minimized precisely when $F$ is a ground state, and $E_0 = \min F[H]$.

The bootstrap lower bound on ground state energy is complementary to the conventional variational upper bounds. Knowing that $E_{lb} \leq E_0 \leq E_{ub}$, the ground state expectation values can be bounded as

$$\text{tr}(\rho_0 O) \geq \min_{F \in A, E_{lb} \leq F[H] \leq E_{ub}} F[O],$$

$$\text{tr}(\rho_0 O) \leq \max_{F \in A, E_{lb} \leq F[H] \leq E_{ub}} F[O].$$

The inequalities (4) can be restrictive when $E_{lb}$ and $E_{ub}$ are close (e.g., see Table II and III).

The method is illustrated with the Hubbard model in one and two dimensions:

$$H = -\sum_{\langle xy \rangle \sigma} c_{x\sigma}^\dagger c_{y\sigma} + U \sum_x n_{x\uparrow} n_{x\downarrow}, \quad (5)$$

where $\langle xy \rangle$ runs over ordered pairs of nearest-neighbor lattice sites, and $c_{x\sigma}$ is the fermion annihilation operator on site $x$ with spin $\sigma = \uparrow, \downarrow$. For simplicity I consider square lattices with unit spacing. The bootstrap works directly in the thermodynamic limit.

The Hamiltonian (5) has discrete lattice translation and rotation symmetries, along with a $U(2)$ global symmetry generated by

$$N = \sum_x (n_{x\uparrow} + n_{x\downarrow}), \quad S_\alpha = \frac{1}{2} \sum_{x \sigma \sigma'} c_{x\sigma}^\dagger (\sigma_\alpha)_{\sigma \sigma'} c_{x\sigma'}, \quad (6)$$

where $\alpha = x, y, z$ and $\sigma_\alpha$ are Pauli matrices. The fermion number $N$, total spin-$z$ component $S_z$, lattice translation and rotation will serve as $C_\alpha$ and $U_{\alpha}$ in (2) for bootstrapping.

As mentioned previously, the choice of $C_1$ and $C_2$ in (2) affects performance of the algorithm. In fermionic lattice models with a local Hamiltonian, such as (5), it is plausible that local operators are more important. Dimensions of the subspaces $C_1$ and $C_2$ are controlled by a positive integer $K$, bounding the degree of locality of operators. The spaces are enlarged when $K$ is increased.

To be more precise, two types of locality are present in (5): $k$-locality ($H$ is a sum of few-body operators) and geometric locality (the interactions are short-ranged). For a string of fermion creation and annihilation operators

$$O = c_{x_1\sigma_1}^\dagger c_{x_2\sigma_2}^\dagger \cdots c_{x_r\sigma_r}^\dagger,$$  

define a locality measure (with respect to a site chosen as the origin)

$$l(O) = r + \sum_{i=1}^r \|x_i\|.$$  

The first term $r$ is the number of fermion operators in (7), counting the degree of $k$-locality. The second term is a sum of geometric $l_1$-norms of the lattice vectors $x_i$. For any positive integer $K$, I choose $C_2$ to be linearly spanned by fermion strings (7) with $l(O) \leq K$, and $C_1$ spanned by the strings that appear in the products of two operators in $C_2$. An ordering of fermion creation and annihilation operators is also employed and only normal ordered strings are considered to avoid unnecessary duplication.

One dimension. — Symmetries imposed in (2) include $C_\alpha = \{H, N, S_\alpha\}$ from (5) and (6), and $U_\alpha = \{T, \Pi\}$. Here $T$ is the lattice translation and $\Pi$ the lattice reflection. For $5 \leq K \leq 10$, $E_{lb}$ in (3) is evaluated and lower bounds the ground state energy. The best bound from $K = 10$ is shown in Table I. Other expectation values are also available, for the functional $F$ that minimizes (3). For example, $D = n_{x\uparrow} n_{x\downarrow}$ in Table I is the double occupancy. Note that $F[D]$ does not necessarily bound the ground state value $(D)_\alpha = \text{tr}(\rho_0 D)$.

Extrapolation to $K = \infty$ is also possible. In Figure 1 expectation values at finite $K$ fit well to the functional form $A + B(\text{dim } C_1)^{-\alpha}$, where $\text{dim } C_1$ is the number of operators in the constraints (2). The fitted $\alpha \approx 0.3$, con-
TABLE II. Bootstrap lower bounds $E_{lb}$ of two-dimensional Hubbard model ground state energies (per site) $E_0$, at fillings $n = 1$ and $n = 0.875$. Solutions from DMET and DMRG are shown for comparison.

| $n = 1$ | $U = 2$ | $U = 4$ | $U = 6$ | $U = 8$ |
|---------|---------|---------|---------|---------|
| $E_{lb}|_{K=7}$ | $-1.221$ | $-0.913$ | $-0.705$ | $-0.565$ |
| $E_{lb}|_{K=\infty}$ | $-$ | $-$ | $-0.66(2)$ | $-0.54(2)$ |
| $E_{DMET}$ | $-1.176(3)$ | $-0.860(3)$ | $-0.656(5)$ | $-0.523(10)$ |
| $E_{DMRG}$ | $-1.176(1)$ | $-0.860(5)$ | $-0.656(1)$ | $-0.524(1)$ |
| $n = 0.875$ | $U = 2$ | $U = 4$ | $U = 6$ | $U = 8$ |
| $E_{lb}|_{K=7}$ | $-1.316$ | $-1.103$ | $-0.963$ | $-0.867$ |
| $E_{lb}|_{K=\infty}$ | $-$ | $-$ | $-0.86(5)$ | $-0.77(3)$ |
| $E_{DMET}$ | $-1.272(16)$ | $-1.031(3)$ | $-0.863(13)$ | $-0.749(7)$ |

TABLE III. Bootstrap bounds $d_{ub}$ of two-dimensional Hubbard model ground state double occupancy (per site) $D = n_{x\uparrow}n_{x\downarrow}$, for the two-dimensional Hubbard model at half filling.

| $n = 1$ | $U = 2$ | $U = 4$ | $U = 6$ | $U = 8$ |
|---------|---------|---------|---------|---------|
| $d_{ub}|_{K=7}$ | $0.160$ | $0.106$ | $0.071$ | $0.049$ |
| $d_{ub}|_{K=\infty}$ | $0.161(6)$ | $0.108(7)$ | $0.072(5)$ | $0.050(3)$ |
| $d_{ub}|_{K=7}$ | $0.224$ | $0.169$ | $0.117$ | $0.079$ |
| $d_{ub}|_{K=\infty}$ | $0.195(14)$ | $-$ | $-$ | $-$ |
| $d_{DMET}$ | $0.1913(4)$ | $0.1261(1)$ | $0.08095(4)$ | $0.05398(7)$ |
| $d_{DMRG}$ | $0.188(1)$ | $0.126(1)$ | $0.0809(3)$ | $0.0539(1)$ |

TABLE IV. Bootstrap upper bounds $m_{ub}$ of ground state staggered magnetization (9) per site, at half filling.

| $n = 1$ | $U = 2$ | $U = 4$ | $U = 6$ | $U = 8$ |
|---------|---------|---------|---------|---------|
| $m_{ub}|_{K=7}$ | $0.194$ | $0.292$ | $0.352$ | $0.383$ |
| $m_{ub}|_{K=\infty}$ | $-$ | $-$ | $-$ | $0.34(2)$ |
| $m_{DMET}$ | $0.133(5)$ | $0.252(9)$ | $0.299(12)$ | $0.318(13)$ |

local observables are constrained by (4). For instance, in the following the DMRG energies at $n = 1$ from [13] are used as $E_{ub}$. Bounds for double occupancy $D$ are shown in Table III, which are restrictive and consistent with other numerics.

As another example, consider the staggered magnetization

$$M = \frac{1}{2} \sum_x (-1)^{x_1+x_2}(n_{x\uparrow} - n_{x\downarrow}),$$

(9)

where $(x_1, x_2)$ are coordinates of $x$. The set of discrete symmetries is reduced to $U_{\alpha} = \{T_{(1,1)}, T_{(1,-1)}, \Pi, R\}$, to allow for nonzero $M$. Upper bounds on $M$ per site are obtained in Table IV. At large $U$ the bound is also consistent with the Heisenberg limit $m \approx 0.307$ [24]. For magnetization the two inequalities in (4) are not independent, as $\min F[M] = - \max F[M]$. 

Discussion.— I have shown that the idea of positivity, which is fundamental in many successful theories, can be employed to solve local lattice models. The bounds are nontrivial checks on other numerics and expand our knowledge of interacting quantum many-body systems.

It would be ideal to have a nonzero lower bound on ground state ordering as well. This is difficult in the current formalism as ground states that do not break symmetries are not ruled out by the constraints. Possibly one should consider two-point functions, by re-introducing non-local few-body operators of interest.

Other directions include generalizing the method to continuous theories, or imposing more constraints on the state (for example, that the state is thermal or a condensate). Also bootstrap bounds on spectral functions, as well as inhomogeneous phases may be useful in constraining low-energy excitations and competing orders in strongly correlated electron systems.

ACKNOWLEDGEMENTS

This work arose from discussions with Sean Hartnoll. The author acknowledges discussions with Sean Hartnoll, Jorrit Kruthoff, Edward Mazenc and Daniel Ranard on related projects.
[1] N. Schuch and F. Verstraete, “Computational complexity of interacting electrons and fundamental limitations of density functional theory,” Nature Physics 5 no. 10, (2009) 732–735.

[2] D. Poland, S. Rychkov, and A. Vichi, “The conformal bootstrap: Theory, numerical techniques, and applications,” Rev. Mod. Phys. 91 (Jan, 2019) 015002.

[3] H. W. Lin, “Bootstraps to strings: Solving random matrix models with positivity,” arXiv:2002.08387 [hep-th].

[4] X. Han, S. A. Hartnoll, and J. Kruthoff, “Bootstrapping matrix quantum mechanics,” arXiv:2004.10212 [hep-th].

[5] S. A. Rice, Reduced-density-matrix mechanics: with application to many-electron atoms and molecules, vol. 165. John Wiley & Sons, 2007.

[6] D. A. Mazziotti, “Two-electron reduced density matrix as the basic variable in many-electron quantum chemistry and physics,” Chemical Reviews 112 no. 1, (01, 2012) 244–262.

[7] T. Baumgratz and M. B. Plenio, “Lower bounds for ground states of condensed matter systems,” New Journal of Physics 14 no. 2, (Feb, 2012) 023027.

[8] B. Verstichel, W. Poelmans, S. De Baerdemacker, S. Wouters, and D. Van Neck, “Variational optimization of the 2DM: Approaching three-index accuracy using extended cluster constraints,” The European Physical Journal B 87 no. 3, (2014) 59.

[9] D. A. Mazziotti, “Enhanced constraints for accurate lower bounds on many-electron quantum energies from variational two-electron reduced density matrix theory,” Phys. Rev. Lett. 117 (Oct, 2016) 153001.

[10] A. Rubio-Garca, J. Dukelsky, D. R. Alcoba, P. Capuzzi, O. B. Oa, E. Ros, A. Torre, and L. Lain, “Variational reduced density matrix method in the doubly-occupied configuration interaction space using four-particle N-representability conditions: Application to the XXZ model of quantum magnetism,” The Journal of Chemical Physics 151 no. 15, (2019) 154104.

[11] J. Hubbard and B. H. Flowers, “Electron correlations in narrow energy bands,” Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences 276 no. 1365, (1963) 238–257.

[12] E. H. Lieb and F. Y. Wu, “Absence of mott transition in an exact solution of the short-range, one-band model in one dimension,” Phys. Rev. Lett. 20 (Jun, 1968) 1445–1448.

[13] Simons Collaboration on the Many-Electron Problem Collaboration, J. P. F. LeBlanc, A. E. Antipov, F. Becca, I. W. Bulik, G. K.-L. Chan, C.-M. Chung, Y. Deng, M. Ferrero, T. M. Henderson, C. A. Jiménez-Hoyos, E. Kozik, X.-W. Liu, A. J. Millis, N. V. Prokof’ev, M. Qin, G. E. Scuseria, H. Shi, B. V. Svistunov, L. F. Tocchio, I. S. Tupitsyn, S. R. White, S. Zhang, B.-X. Zheng, Z. Zhu, and E. Gull, “Solutions of the two-dimensional hubbard model: Benchmarks and results from a wide range of numerical algorithms,” Phys. Rev. X 5 (Dec, 2015) 041041.

[14] B.-X. Zheng, C.-M. Chung, P. Corboz, G. Ehlers, M.-P. Qin, R. M. Noack, H. Shi, S. R. White, S. Zhang, and G. K.-L. Chan, “Stripe order in the underdoped region of the two-dimensional hubbard model,” Science 358 no. 6367, (2017) 1155–1160.

[15] E. W. Huang, C. B. Mendl, S. Liu, S. Johnston, H.-C. Jiang, B. Moritz, and T. P. Devereaux, “Numerical evidence of fluctuating stripes in the normal state of high-Tc cuprate superconductors,” Science 358 no. 6367, (2017) 1161–1164.

[16] P. W. Anderson, “Limits on the energy of the antiferromagnetic ground state,” Phys. Rev. B 83 (Sep, 1951) 1260–1260.

[17] R. Valentí, J. Stolze, and P. J. Hirschfeld, “Lower bounds for the ground-state energies of the two-dimensional hubbard and t-J models,” Phys. Rev. B 43 (Jun, 1991) 13743–13746.

[18] R. Valentí, C. Gros, P. J. Hirschfeld, and W. Stephan, “Rigorous bounds for ground-state properties of correlated fermi systems,” Phys. Rev. B 44 (Dec, 1991) 13203–13212.

[19] B. O’Donoghue, E. Chu, N. Parikh, and S. Boyd, “Conic optimization via operator splitting and homogeneous self-dual embedding,” Journal of Optimization Theory and Applications 169 no. 3, (June, 2016) 1042–1068.

[20] B. O’Donoghue, E. Chu, N. Parikh, and S. Boyd, “SCS: Splitting conic solver, version 2.1.2.” https://github.com/cvxgrp/scs, Nov., 2019.

[21] G. Knizia and G. K.-L. Chan, “Density matrix embedding: A simple alternative to dynamical mean-field theory,” Phys. Rev. Lett. 109 (Nov, 2012) 186404.

[22] B.-X. Zheng and G. K.-L. Chan, “Ground-state phase diagram of the square lattice Hubbard model from density matrix embedding theory,” Phys. Rev. B 93 (Jan, 2016) 035126.

[23] S. R. White, “Density matrix formulation for quantum renormalization groups,” Phys. Rev. Lett. 69 (Nov, 1992) 2863–2866.

[24] A. W. Sandvik, “Finite-size scaling of the ground-state parameters of the two-dimensional Heisenberg model,” Phys. Rev. B 56 (Nov, 1997) 11678–11690.