A variational lower bound on the ground state of a many-body system and the squaring parametrization of density matrices

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Abstract. A variational *upper* bound on the ground state energy $E_{\rm gs}$ of a quantum system, $E_{\rm gs} \leq \langle \Psi | H | \Psi \rangle$, is well-known (here H is the Hamiltonian of the system and Ψ is an arbitrary wave function). Much less known is the variational *lower* bound on the ground state of a many-body translation-invariant lattice system with the Hamiltonian $H = \sum_{i=1}^{N} h_i$, where local terms h_i can be obtained from h_1 by translations (and rotations, for lattices in two and three dimensions). This bound reads $E_{\rm gs} \geq N \operatorname*{tr}_{\rho \in \mathbb{M}} h_1 \rho$, where $\mathbb{M}$ is some wisely chosen set of reduced density matrices ρ. The implementation of this latter variational principle is hampered by the difficulty of parameterizing the set $\mathbb{M}$, which is a necessary prerequisite for a variational procedure. The root cause of this difficulty is the nonlinear positivity constraint $\rho > 0$ which is to be satisfied by a density matrix. The squaring parametrization of the density matrix, $\rho = \tau^2 / \operatorname{tr} \tau^2$, where τ is an arbitrary (not necessarily positive) Hermitian operator, accounts for positivity automatically. We discuss how the squaring parametrization can be utilized to find variational lower bounds on ground states of translation-invariant many-body systems. As an example, we consider the Heisenberg model of spins 1/2 in one and two dimensions.

References

[1] Nikolay Il'in, Elena Shpagina, Filipp Uskov, Oleg Lychkovskiy. Squaring parametrization of constrained and unconstrained sets of quantum states, J. Phys. A: Math. Theor. 51, 085301 (2018).