Lower Bound for the Ground-State Energy Density of a 1D Quantum Spin System

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We present a simple method to calculate systematic lower bounds for the ground-state energy density of a 1D quantum spin system.

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The ground-state energy is a quantity of fundamental interest in the study of quantum spin systems. For example, nonanalytic behaviour of the ground-state energy as a parameter in the hamiltonian is varied is a canonical signature of a quantum phase transition [1]. The ground-state energy also occupies a central role in quantum computational complexity theory: the problem of calculating a good approximation to the ground-state energy for a class of 2D spin systems is complete for the complexity class QMA, which is the quantum analogue of NP [2, 3, 4].

Obviously, because of the QMA-completeness results of Kempe et. al. [3] and Oliveira and Terhal [4] we expect that the ground-state energy is, in general, extremely difficult to approximate. However, as these results only pertain to highly disordered/frustrated 2D systems, there is some hope that it might be possible to efficiently calculate approximations to the ground-state energy for 1D systems and regular 2D systems.

This hope has been partially vindicated by the development of the density matrix renormalisation group (DMRG) (see [5] and references therein for a description of the DMRG and relatives). The DMRG provides an apparently efficient algorithm to calculate the ground-state energy and other local ground-state properties for 1D quantum spin systems. An exciting extension of the DMRG to 2D quantum spin systems was recently developed by [6].

Unfortunately the DMRG cannot certify that the estimate it provides for the ground-state energy is close to the real value. The reason is that there is no way to rule out the possibility that the DMRG has become stuck in a local minima. For this reason, if a promise that the calculated ground-state energy is close to the correct value is required, then it is vital to either develop algorithms which provide an estimate on the distance from optima, or, because the DMRG estimates are always upper bounds, provide a method to calculate systematic lower bounds for the ground-state energy.

There has been some previous work on lower bounds for the ground-state energy: the most important general method which has been proposed so far is due to Anderson [7]. This method has been developed further and applied to many situations, see eg. [8]. The Anderson bound, while nontrivial, is suboptimal; as we’ll see later there exist systems for which the Anderson bound cannot be systematically improved fast enough to be useful practically.

In this Letter we describe a simple method to calculate systematic lower bounds for the ground-state energy density (the ground-state energy per particle) of a 1D spin system. For general local 1D systems it is an efficient numerical procedure to extract the lower bound. For some systems our method is purely analytic. As a test we apply our method to calculate a lower bound for ground-state energy density of the XY model. We also apply our method to find a lower bound for the average ground-state energy density of the disordered heisenberg model. Finally, we construct systems for which the Anderson bound cannot be improved efficiently, yet our method provides the exact answer.

We consider quantum systems defined on a set of vertices $V$ with a finite dimensional Hilbert space $\mathcal{H}_x$, i.e. a quantum spin, attached to each vertex $x \in V$. We always assume that $V$ is finite owing to the standard difficulties [9, 10] in defining a thermal state for infinite quantum spin systems. While we take the limit $n \to \infty$ we understand that this limit is purely formal and, strictly speaking, our results pertain only to the situation where $n$ is large but finite.

We will, for the sake of clarity, introduce and describe our results for a ring $C$ of $n$ distinguishable spin-$\frac{1}{2}$ particles. Thus, the Hilbert space $\mathcal{H}_C$ for our system is given by $\mathcal{H}_C = \bigotimes_{j=0}^{n-1} \mathbb{C}^2$.

We now introduce the family $H_n$ of local hamiltonians we are going to focus on. To define our family we’ll initially fix some two-spin interaction term $G$ which has bounded norm: $\|G\| \leq \text{const.}$ (Note that we can, and will, accommodate next-nearest neighbour interactions etc. by increasing the local dimension of the spins, i.e. by blocking neighbouring spins.) We write the spectral decomposition of $G$ as $G = \sum_{j=0}^{n-1} \lambda_j |\lambda_j\rangle\langle\lambda_j|$. By a trivial rescaling of the zero point of energy we’ll always take $\lambda_{\min}(G) = \lambda_0 = 0$. Our family $H_n$ of local quantum systems is then defined by

$$H_n = \sum_{j=0}^{n-1} G_j,$$

where $G_j$ is a translate of $G$, i.e., it acts nontrivially on spins $j$ and $j+1$ as $G$, and as the identity elsewhere.

Now, it is clear that the ground-state energy eigenvalue $E_0 \geq 0$ of $H$ will, in general, be strictly positive. In this
case, by using approximate eigenvectors on blocks, it is relatively straightforward to argue that \( E_0 \) scales as \( E_0 \sim c_0 + e_0 n \), where \( c_0 \) and \( e_0 \) are constants. Typically \( c_0 < 0 \) and \( e_0 > 0 \). Because of this scaling it makes sense to talk about the ground-state energy density \( E_0 / n \rightarrow e_0 \). It is this quantity we wish to bound.

The central part of our argument relies on the Golden-Thompson inequality \([11, 12]\) (this is Corollary IX.3.6 in \([13]\)):

\[
\text{tr}(e^{A+B}) \leq \text{tr}(e^A e^B),
\]

where \( A \) and \( B \) are hermitian operators. To apply the Golden-Thompson inequality we divide the hamiltonian \( H \) into two pieces:

\[
H = A + B,
\]

where \( A = \sum_{j=0}^{n/2-1} G_{2j} \) and \( B = \sum_{j=0}^{n/2-1} G_{2j+1} \).

Our argument works by first applying the Golden-Thompson inequality Eq. \((2)\) to the thermal state \( e^{-\beta H} \) using the partition Eq. \((3)\). This gives us the inequality

\[
\mathcal{Z}(\beta) = \text{tr}(e^{-\beta H}) \leq \text{tr}(e^{-\beta A} e^{-\beta B}),
\]

where \( \mathcal{Z}(\beta) \) is the partition function. Next we study the expression \( e^{-\beta A} e^{-\beta B} \). We begin by writing

\[
e^{-\beta A} e^{-\beta B} = \sum_{\alpha, \beta=0}^3 M(\beta)_{\alpha \beta} \sigma^\alpha \otimes \sigma^\beta,
\]

where \( \sigma^\alpha = \{ 0 \ 1 \; 1 \ 0 \; (0 \ 1) \; (1 \ 0) \; (0 \ -1) \; (1 \ 0) \} \), is the vector of Pauli sigma matrices.

We use this expansion to derive an expression for \( e^{-\beta A} e^{-\beta B} \):

\[
e^{-\beta A} e^{-\beta B} = \sum_{\alpha, \beta=0}^3 M(\beta)_{\alpha \beta} \sigma^\alpha \otimes \sigma^\beta.
\]

This gives us the inequality

\[
\text{tr}(e^{-\beta H}) \leq 2^n \text{tr}(M(\beta)^n).
\]

Substituting the expansion Eq. \((6)\) into Eq. \((4)\) gives us

\[
\text{tr}(e^{-\beta H}) \leq 2^n \text{tr}(M(\beta)^n).
\]

The next step is to bound the partition function from below:

\[
e^{-\beta E_0} \leq \text{tr}(e^{-\beta H}) \leq 2^n \text{tr}(M(\beta)^n).
\]

We now observe, thanks to the positivity of \( \text{tr}(M(\beta)^n) \) for all \( n \in \mathbb{N} \), that

\[
\text{tr}(M(\beta)^n) \leq D \| M(\beta) \|^n_c,
\]

where \( D \) is the dimension of \( M \). Applying this inequality to Eq. \((8)\) and taking logs gives us

\[
-\beta E_0 \leq \log(D) + n \log(\|2M(\beta)\|).
\]

After rearranging we obtain the following inequality for the ground-state energy density:

\[
E_0 / n \geq -\log(D)/(\beta n) - \log(\|2M(\beta)\|)/\beta,
\]

for all \( \beta \in [0, \infty) \).

We will be interested in the large-\( n \) limit where \( n \gg 1/\beta \). In this case we can ignore the first contribution on the RHS of Eq. \((11)\). Thus we obtain our fundamental inequality

\[
E_0 / n \geq -\inf_{\beta \in [0, \infty)} \log(\|2M(\beta)\|)/\beta
\]

In principle our fundamental inequality Eq. \((12)\) provides an analytic lower bound for \( E_0 / n \). In practice, however, we need to resort to numerical evaluation of the RHS. This is an efficient procedure (in \( n \)) and, thanks to the continuity of \( \log(\|2M(\beta)\|)/\beta \) as a function of \( \beta \in [0, \infty) \), provides a certified lower bound for \( E_0 / n \).

Can the lower bound Eq. \((12)\) be improved? There are at least two ways to proceed. The first method is to combine \( l \) contiguous spins into blocks \( \Lambda \) and regard each block \( \Lambda \) as a fundamental spin (of dimension \( 2^l \)). We similarly block the hamiltonian \( H \), which leads to a new nearest-neighbour hamiltonian for the bigger spins. We can then apply the procedure we outlined above, albeit using a different operator basis from standard operator basis. This will lead to a new lower bound. It is obvious that this procedure cannot lead to a bound which is any worse: after all, by taking \( l = n \) we recover the exact value of \( E_0 \).

The second procedure is to look for decompositions of \( H \) where \( H = \sum_{j=0}^{n-1} H_j \) and where \( H_j \) has a larger minimum eigenvalue. We then apply the procedure described above using \( H_j \) instead of \( H_j \). We’ll describe a systematic procedure to obtain such decompositions in a future paper.
There are several obvious generalisations of our method. The first generalisation is to calculate $e^{-\beta H_x}$ for very large blocks $\Lambda$ of spins via numerical RG methods such as those described in [15] and [16]. In this case we must put error bars on the calculated lower bound because of the truncations required by the methods of [15] and [16]. Applying this technique can give us, in principle, arbitrarily good lower bounds to the ground-state energy density.

The second generalisation is to quantum spin systems in dimensions higher than one. In this case it is straightforward to apply our argument to blocks of spins and thus derive an expression for the upper bound which resembles the tensor contraction patterns investigated in [6] and [17]. Applying the methods described there to approximate such tensor contraction patterns will allow us to derive lower bounds for the ground state energy of finite higher-dimensional spin systems.

The third generalisation applies to disordered systems. It is entirely straightforward to allow the interaction $G$ to vary from site to site: the method described above applies with essentially no change to such systems. However, in this case, we need to average the lower bound over the ensemble of possible interactions. In principle this can be done analytically for several models. To illustrate the utility of our lower bound for disordered systems we apply this technique to the random antiferromagnetic heisenberg model:

$$H = \sum_{k \in \mathbb{Z}} J_k \sigma_k \cdot \sigma_{k+1},$$  \hspace{1cm} (13)

where $J_k$ is a random variable with probability distribution function $\mu(x)$. Applying our bound Eq. (12), appropriately modified for disordered systems, and averaging over the measure $d\mu(x)$ gives us the following lower bound for the expected ground-state energy density:

$$\langle e_0 \rangle \geq -3\langle x \rangle + \log(2)/\beta - \int d\mu(x) \frac{\log(1 + 3e^{-4\beta x})}{\beta},$$  \hspace{1cm} (14)

for all $\beta \in (0, \infty)$, where $\langle A(x) \rangle = \int d\mu(x) A(x)$. Choosing, for example, $d\mu(x) = e^{-x^2}/N$, where $N$ is a normalisation, and choosing $x \in [0, \infty)$ provides us with the (numerically obtained) lower bound $\langle e_0 \rangle \geq -0.833610$. Compare this lower bound with the Anderson bound [7]: $\langle e_0 \rangle \geq -1.32934$.

Finally, we say a couple of words about the optimality of our approach. Consider the interaction term

$$G = -|01\rangle\langle 01| + 2|10\rangle\langle 10| + 3|11\rangle\langle 11|. \hspace{1cm} (15)$$

Now the Anderson bound applied to $H = \sum_{j=1}^{n-1} G_j$ yields a lower bound for the ground-state energy density given by $-1$ whereas the method we’ve developed here yields the exact answer: $e_0 = 0$. Even after blocking $m$ spins the Anderson lower bound is still only $-1/m$.

The decomposition Eq. (6) and subsequent derivation are strongly reminiscent of DMRG-type methods based on matrix product states (MPS) [18]. It is certainly true that methods for the ground-state energy based on MPS reduce to variational problems over a restricted class of vectors in hilbert space and thus must have a well defined lagrangian dual which would, at least in principle, provide lower bounds for the ground-state energy density. (Further investigation of this dual problem will be reported elsewhere). It is currently unclear what, if any, connection our method has to this dual problem.

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