Computing local properties in the trivial phase

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Abstract

A translation-invariant gapped local Hamiltonian is in the trivial phase if it can be connected to a completely decoupled Hamiltonian with a smooth path of translation-invariant gapped local Hamiltonians. For the ground state of such a Hamiltonian, we show that the expectation value of a local observable can be computed in time poly(1/δ) in one spatial dimension and e^{poly log(1/δ)} in two and higher dimensions, where δ is the desired (additive) accuracy. The algorithm applies to systems of finite size and in the thermodynamic limit. It only assumes the existence but not any knowledge of the path.

1 Introduction and background

Computing the ground-state expectation value of a local observable in quantum many-body systems is a fundamental problem in condensed matter physics. We consider this problem for translation-invariant gapped local Hamiltonians in systems of finite size and in the thermodynamic limit. Here, “gapped” means that the energy gap (defined as the energy difference between the unique ground state and the first excited eigenstate) is lower bounded by a positive constant independent of the system size. For notational simplicity, we first work with a chain of N spins, each of which has constant local dimension. In Section 3 we extend the results to two and higher spatial dimensions.

It is straightforward to define translation-invariant local Hamiltonians in the thermodynamic limit N → +∞. Without loss of generality, we only consider nearest-neighbor interactions. Let \( h_1 \) with \( \| h_1 \| \leq 1 \) be a Hermitian operator acting on the first two spins. Let \( T \) be the (unitary) lattice translation operator so that \( h_j := T^{j-1} h_1 T^{-(j-1)} \) acts on the \( j \)th, \( (j+1) \)th spins. For concreteness, we use open boundary conditions (we will discuss periodic boundary conditions later) and define

\[
H = \left\{ H^{(N)} \right\}, \quad H^{(N)} := \sum_{j=1}^{N-1} h_j
\]

as a sequence of translation-invariant local Hamiltonians: one for each system size \( N \).

Do the ground-state properties of \( H^{(N)} \) depend smoothly on the system size \( N \) and become well defined in the thermodynamic limit \( N \to +\infty \)? Not always. For example, the ground-state energy (as a function of \( N \)) can encode the solution of a computationally intractable problem [12, 13, 3].

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The problem of whether a constant energy gap persists in the thermodynamic limit is undecidable \[9, 2\]. In size-driven quantum phase transitions, the ground-state properties change abruptly as \(N\) crosses the critical system size \(N_c\) \[3\]. There is good evidence that even under the assumption of a constant energy gap, the ground-state expectation value of a local observable may not always be computed in time independently of \(N\) \[10, 22\].

In this paper, we consider the case that \(H\) is in the trivial phase.

**Definition 1** (trivial phase; see, e.g., Refs. \[7, 29, 16, 23\]). \(H = \{H^{(N)}\}\) is in the trivial phase if there exists a smooth path \(H(s) = \{H^{(N)}(s)\}\) of translation-invariant local Hamiltonians

\[
H^{(N)}(s) = \sum_{j=1}^{N-1} h_j(s), \quad h_j(s) := T_j^{-1} h_1(s) T_j^{-(j-1)}, \quad 0 \leq s \leq 1
\]

such that

- \(H^{(N)}(0)\) is a completely decoupled Hamiltonian so that its ground state is a product state.
- \(H^{(N)}(1) = H^{(N)}\).
- \(||h_1(s)|| \leq 1\) and \(||dh_1(s)/ds|| \leq 1\).
- The energy gap of \(H^{(N)}(s)\) is lower bounded by a positive constant \(\epsilon\) for any \(0 \leq s \leq 1\) and \(N \geq N_0\), where \(N_0\) is a constant.

It is widely believed (and argued using uniform matrix product states \[11, 28\]) that the trivial phase is the only gapped phase in one-dimensional translation-invariant systems \[8, 29\]. Therefore, being in the trivial phase is a very mild assumption in one spatial dimension.

## 2 One dimension

Throughout this paper, asymptotic notations are used extensively. Let \(f, g : \mathbb{R}^+ \to \mathbb{R}^+\) be two functions. One writes \(f(x) = O(g(x))\) if and only if there exist positive numbers \(M, x_0\) such that \(f(x) \leq Mg(x)\) for all \(x > x_0\); \(f(x) = \Omega(g(x))\) if and only if there exist positive numbers \(M, x_0\) such that \(f(x) \geq Mg(x)\) for all \(x > x_0\). To simplify the notation, we use a tilde to hide a polylogarithmic factor, e.g., \(\tilde{O}(f(x)) := O(f(x) \text{poly} |\log f(x)|)\).

Let \(A_1\) with \(||A_1|| \leq 1\) be a local operator acting on the first few spins, and \(A_j := T_j^{-1} A_1 T_j^{-(j-1)}\) be the lattice-translated copy of \(A_1\). Let \(\langle \hat{O} \rangle_N := \langle \hat{\psi}^{(N)} | \hat{O} | \hat{\psi}^{(N)} \rangle\) be the expectation value of an operator in the ground state \(\hat{\psi}^{(N)}\) of \(H^{(N)}\).

**Lemma 1** (open boundary conditions). Suppose that \(H = \{H^{(N)}\}\) is in the trivial phase. Then,

\[
\left| \langle A_j \rangle_N - \langle A_j \rangle_{N+1} \right| = e^{-\tilde{\Omega}(N-j)}, \quad \text{(3)}
\]

\[
\left| \langle A_j \rangle_N - \langle A_{j+1} \rangle_N \right| = e^{-\tilde{\Omega}(\min\{j,N-j\})}, \quad \text{(4)}
\]

Therefor, both \(\lim_{N \to +\infty} \langle A_j \rangle_N\) and \(\lim_{N \to +\infty} \langle A_{[\alpha,N]} \rangle_N\) are well defined, where \(0 < \alpha < 1\) is a constant and \([\cdots]\) denotes the floor function. Furthermore, the value of the latter limit is independent of \(\alpha\).

**Proof.** We use the technique of quasi-adiabatic continuation, which was originally due to Hastings \[14, 19\] and subsequently developed in Refs. \[27, 15, 1\]. Combining with the Lieb-Robinson bound \[24, 28, 17, 30\], this technique has applications in proving, e.g., stability of topological order \[6, 5, 25\] and quantization of the Hall conductance \[18\].
Following Ref. [10], we give a high-level overview of quasi-adiabatic continuation. Define

\[
D^{(N)}(s) = \sum_{j=1}^{N-1} D_j^{(N)}(s), \quad D_j^{(N)}(s) = i \int_{-\infty}^{+\infty} f(t) e^{iH^{(N)}(s)t} \frac{dh_j(s)}{ds} e^{-iH^{(N)}(s)t} dt,
\]

where the “filter function” \( f(t) \) is purely imaginary so that \( D^{(N)}(s) \) is Hermitian. Let \( \psi^{(N)}(s) \) be the ground state of \( H^{(N)}(s) \). Reference [15] explicitly constructed \( f(t) \) such that

\[
\frac{d\psi^{(N)}(s)}{ds} = -iD^{(N)}(s)\psi^{(N)}(s),
\]

\[
|f(t)| = e^{-\Omega(t/\log^{1.001} t)} = e^{-\tilde{\Omega}(t)}.
\]

The first equation allows us to interpret \( D^{(N)}(s) \) as a time-dependent Hamiltonian, whose dynamics generates the state \( \psi^{(N)}(s) \) from \( \psi^{(N)}(0) \). Let \( B(j, r) \) be the radius-\( r \) neighborhood of the \( j \)th spin. Choosing an appropriate constant \( c \), we split the integral (5) into two terms:

\[
D_j^{(N)}(s) = i \int_{|t| \leq cr} \cdots + i \int_{|t| > cr} \cdots.
\]

The first term is approximately supported on \( B(j, r) \) due to the Lieb-Robinson bound for \( H^{(N)}(s) \), and second term is negligible due to the fast decay \( (7) \) of \( f(t) \). Hence, \( D_j^{(N)}(s) \) is local in the sense that

\[
\left\| D_j^{(N)}(s) - D_j^{(N)}(s) \right\|_{B(j, r)} = e^{-\tilde{\Omega}(r)}, \quad \forall j, s,
\]

where \( D_j^{(N)}(s)|_{B(j, r)} \) is the best approximation of \( D_j^{(N)}(s) \) supported on \( B(j, r) \). The locality \( (9) \) of \( D_j^{(N)}(s) \) implies that the dynamics generated by \( D^{(N)}(s) \) also satisfies a Lieb-Robinson bound [15]. A similar argument shows that

\[
\left\| D_j^{(N)}(s) - D_j^{(N+1)}(s) \right\| = e^{-\tilde{\Omega}(N-j)}.
\]

Let

\[
U^{(N)}(s) := S'e^{-i \int_0^s D^{(N)}(s') ds'} = S'e^{-i \int_0^s \sum_{k=1}^{N-1} D_k^{(N)}(s') ds'},
\]

where \( S' \) is the \( s' \)-ordering operator. The thermodynamic limit of quasi-adiabatic continuation exists [11] in the sense that

\[
\left\| U^{(N)}(s)A_jU^{(N)}(s) - U^{(N+1)}(s)A_jU^{(N+1)}(s) \right\| = e^{-\tilde{\Omega}(N-j)}.
\]

Indeed, the difference between \( D_k^{(N)}(s') \) and \( D_k^{(N+1)}(s') \) for \( k \leq (j + N)/2 \) is controlled by Eq. (10). For \( k > (j + N)/2 \), the effects of \( D_k^{(N)}(s') \) and \( D_k^{(N+1)}(s') \) are negligible because the dynamics generated by \( D^{(N)}(s') \) satisfies a Lieb-Robinson bound.

Equation (3) follows from Eq. (12) and the fact that \( \psi^{(N)}(0) \) is the reduced state of \( \psi^{(N+1)}(0) \) on the first \( N \) spins. Equation (14) is obtained by using Eq. (3) twice: In a chain of \( N \) spins, we add an \((N+1)\)th spin and delete the first spin, introducing errors of \( e^{-\tilde{\Omega}(N-j)} \) and \( e^{-\tilde{\Omega}(j)} \), respectively. The “therefore” and “furthermore” parts of Lemma 1 are straightforward consequences of Eqs. (3), (4).
Corollary 1. Suppose that $H = \{H^{(N)}\}$ is in the trivial phase. The ground-state energy density converges as
\[
\frac{\langle H^{(N)} \rangle_{N}}{N-1} - \lim_{N' \to +\infty} \frac{\langle H^{(N')} \rangle_{N'}}{N' - 1} = O(1/N).
\] (13)

Proof. It follows from
\[
\begin{align*}
\left| \frac{\langle H^{(N)} \rangle_{N}}{(N - 1)} - \frac{\langle H^{(N+1)} \rangle_{N+1}}{N} \right| &= \sum_{j=1}^{[N/2]-1} \frac{|\langle h_j \rangle_{N} - \langle h_j \rangle_{N+1}|}{N-1} + \frac{\sum_{j=1}^{[N/2]} |\langle h_j \rangle_{N} - \langle h_{j+1} \rangle_{N+1}|}{N-1} \\
&+ \sum_{j=1}^{[N/2]} \frac{|\langle h_{j+1} \rangle_{N+1} - \langle h_{[N/2]} \rangle_{N+1}|}{(N-1)N} + \sum_{j=1}^{N} \frac{|\langle h_{j} \rangle_{N+1} - \langle h_{[N/2]} \rangle_{N+1}|}{(N-1)N} \\
&\leq e^{-\tilde{\Omega}(N)} + e^{-\tilde{\Omega}(N)} + \sum_{j=1}^{[N/2]-1} \frac{je^{-\tilde{\Omega}(-j)}}{(N-1)N} + \sum_{j=1}^{N} \frac{(N+1-j)e^{-\tilde{\Omega}(-(N+1-j))}}{(N-1)N} = O(1/N^2). 
\end{align*}
\] (14)

Theorem 1. Suppose that $H = \{H^{(N)}\}$ is in the trivial phase. Then, $\langle A_j \rangle_N$ for any $j, N$ and the limits $\lim_{N \to +\infty} \langle A_j \rangle_N$, $\lim_{N \to +\infty} \langle A_{\alpha N} \rangle_N$ for any $0 < \alpha < 1$ can be computed to additive accuracy $\delta$ in time $\text{poly}(1/\delta)$, where the degree of the polynomial is an absolute constant independent of the energy gap.

Proof. Let $B(j, r)$ be the radius-$r$ neighborhood of the $j$th spin. Lemma 1 implies that the expectation value of $A_j$ in the ground state of
\[
H^{(N)}|_{B(j, r)} := \sum_{j \in B(j, r)} h_j
\] (15)
is an approximation to $\langle A_j \rangle_N$ with error $e^{-\tilde{\Omega}(r)}$. (Similarly, $\lim_{N \to +\infty} \langle A_j \rangle_N$ can be computed from $H^{(N \to +\infty)}|_{B(j, r)}$, which is supported on a subsystem of finite size.) To achieve additive accuracy $\delta$, it suffices to choose $r = \tilde{O}(\log(1/\delta))$. Exactly diagonalizing $H^{(N)}|_{B(j, r)}$ would result in an algorithm with running time $e^{O(r)} = e^{\tilde{O}(\log(1/\delta))}$, which is already close to but still worse than $\text{poly}(1/\delta)$. Since $H^{(N)}|_{B(j, r)}$ has a constant energy gap, we can use the algorithm in Ref. 20. The running time of the algorithm is polynomial in the (sub)system size and inverse precision: $\text{poly}(r, 1/\delta) = \text{poly}(1/\delta)$, where the degree of the polynomial is an absolute constant independent of the energy gap.

Remark. It may be interesting to compare Theorem 1 with a result of Ref. 21. Only assuming a constant energy gap (not translational invariance or being in the trivial phase), this reference gives an algorithm that computes the ground-state energy density $\langle H^{(N)} \rangle_N/(N - 1)$ to additive accuracy $\delta$ in time $\text{poly}(1/\delta)$.
2.1 Periodic boundary conditions

In this subsection only, we consider periodic boundary conditions. For Definition \[ \text{[I]} \] (of the trivial phase), the only modification is that the translation-invariant gapped local Hamiltonians \( H(s) = \{ H^{(N)}(s) \} \) in the smooth path should also use periodic boundary conditions. Equation \[ \text{[I]} \] becomes trivial: The left-hand side is identically 0 due to the translational invariance of the ground state. The proof of the following lemma is essentially the same as that of Lemma \[ \text{[I]} \]

**Lemma 2.** Suppose that \( H = \{ H^{(N)} \} \) is in the trivial phase. Then,

\[
|\langle A_j \rangle_N - \langle A_j \rangle_{N+1}| = e^{-\tilde{\Omega}(N)}.
\]

(16)

Therefore, \( \lim_{N \to +\infty} \langle A_j \rangle_N \) is well defined.

**Corollary 2.** Suppose that \( H = \{ H^{(N)} \} \) is in the trivial phase. Then,

\[
|\langle h_j \rangle_N - \lim_{N' \to +\infty} \langle h_j \rangle_{N'}| = e^{-\tilde{\Omega}(N)}.
\]

(17)

This corollary provides a rigorous justification of the empirical observation that in many one-dimensional translation-invariant gapped systems with periodic boundary conditions, the ground-state energy density converges (almost) exponentially in the system size \( N \). In contrast, with open boundary conditions Corollary \[ \text{[I]} \] shows that the scaling is only \( O(1/N) \) due to boundary effects.

Theorem \[ \text{[I]} \] remains valid for periodic boundary conditions without any modification.

3 Higher dimensions

It is very straightforward to extend the results to two and higher spatial dimensions. For notational simplicity and without loss of generality, we consider a two-dimensional square lattice of size \( N_x \times N_y \). The thermodynamic limit is defined as a sequence of lattices with growing size \( N_x, N_y \to +\infty \). There is one spin at each lattice site, labeled by \( (j_x, j_y) \) with \( 1 \leq j_x \leq N_x \) and \( 1 \leq j_y \leq N_y \). We use open boundary conditions and define \( H = \{ H^{(N_x,N_y)} \} \) as a sequence of translation-invariant local Hamiltonians: one for each system size \( N_x \times N_y \). Let \( T_x, T_y \) be the lattice translation operators in the \( x, y \) directions, respectively. Let \( A_{1,1} \) with \( \| A_{1,1} \| \leq 1 \) be a local operator supported in a small neighborhood of site \((1,1)\), and

\[
A_{j_x,j_y} := T_y^{j_y-1} T_x^{j_x-1} A_{1,1} T_x^{-(j_x-1)} T_y^{-(j_y-1)}.
\]

(18)

be a local operator supported in a small neighborhood of site \((j_x,j_y)\). Let \( \langle \hat{O} \rangle_{N_x,N_y} \) be the expectation value of an operator \( \hat{O} \) in the ground state of \( H^{(N_x,N_y)} \).

Since quasi-adiabatic continuation works in any dimension, Lemma \[ \text{[I]} \] directly generalizes to

**Lemma 3 (open boundary conditions).** Suppose that \( H = \{ H^{(N_x,N_y)} \} \) is in the trivial phase. Then,

\[
|\langle A_{j_x,j_y} \rangle_{N_x,N_y} - \langle A_{j_x,j_y} \rangle_{N_x+1,N_y}| = e^{-\tilde{\Omega}(N_x-j_x)},
\]

(19)

\[
|\langle A_{j_x,j_y} \rangle_{N_x,N_y} - \langle A_{j_x,j_y} \rangle_{N_x,N_y+1}| = e^{-\tilde{\Omega}(N_y-j_y)},
\]

(20)

\[
|\langle A_{j_x,j_y} \rangle_{N_x,N_y} - \langle A_{j_x+1,j_y} \rangle_{N_x,N_y}| = e^{-\tilde{\Omega}(\min(j_x,N_x-j_x))},
\]

(21)

\[
|\langle A_{j_x,j_y} \rangle_{N_x,N_y} - \langle A_{j_x,j_y+1} \rangle_{N_x,N_y}| = e^{-\tilde{\Omega}(\min(j_y,N_y-j_y))}.
\]

(22)

Therefore, both \( \lim_{N_x,N_y \to +\infty} \langle A_{j_x,j_y} \rangle_{N_x,N_y} \) and \( \lim_{N_x,N_y \to +\infty} \langle A_{[\alpha_x,N_x],[\alpha_y,N_y]} \rangle_{N_x,N_y} \) are well defined (and do not depend on the order of limits), where \( 0 < \alpha_x, \alpha_y < 1 \) are constants. Furthermore, the value of the latter limit is independent of \( \alpha_x, \alpha_y \).

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Theorem 2. Suppose that $H = \{H^{(N_x,N_y)}\}$ is in the trivial phase. Then, $\langle A_{j_x,j_y} \rangle_{N_x,N_y}$ for any $j_x,j_y,N_x,N_y$ and the limits $\lim_{N_x,N_y \to +\infty} \langle A_{j_x,j_y} \rangle_{N_x,N_y}$, $\lim_{N_x,N_y \to +\infty} \langle A_{[\alpha_x N_x],[\alpha_y N_y]} \rangle_{N_x,N_y}$ for any $0 < \alpha_x, \alpha_y < 1$ can be computed to additive accuracy $\delta$ in time $e^{\tilde{O}(\log^2(1/\delta))}$.

Proof. We exactly diagonalize the Hamiltonian restricted to a $r \times r$ neighborhood of site $(j_x,j_y)$. Lemma 3 implies that $r = \tilde{O}(\log(1/\delta))$ suffice, and the running time is $e^{\tilde{O}(r^2)} = e^{\tilde{O}(\log^2(1/\delta))}$. \qed

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