Lower energy bounds for quantum lattice Hamiltonians

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Abstract
We derive general lower energy bounds for the ground state energy of any translationally invariant quantum lattice Hamiltonian. The bounds are given by the ground state energy of renormalized Hamiltonians on finite clusters.

1 Introduction
When computing the low energy eigenstates for some quantum Hamiltonian, $H$, one usually extracts an energy estimate by calculating the expectation of $H$ for some approximate wavefunction. In the case of the ground state this estimate also provides an upper bound on the energy. The calculation is usually repeated with systematically improved wavefunction approximations and the final result is determined by extrapolation. While in principle this procedure should work, in practice computational difficulties can block improvement beyond some point. One common culprit is the fermion sign problem. Although the sign problem can be delayed with some success, as shown in [1], in the end it will eventually lead to exponential scaling of computational effort. In such cases it is quite useful to have some idea of how far a given estimate is from the exact answer.

Since in most cases the result in hand provides an upper bound to the ground state energy, what is needed is a reasonably accurate lower bound. In this letter we state and derive a general lower bound for the ground state energy of any translationally invariant lattice Hamiltonian. Our result is very general and applies to any number of dimensions, size of lattice, type of particle, or form of local interactions. In particular this includes single-site terms, nearest and next-nearest neighbor hoppings, and gauge plaquettes. The only restriction is that the interactions are localized and do not extend throughout the entire lattice. The lower bound is stated in terms of the ground state energy for a renormalized Hamiltonian defined on a cluster subset. As we find in the example described below, the error appears to scale as the ratio of the boundary size to the bulk
size of the cluster. Since the lower bound is defined on clusters, it is most convenient for position-space computational schemes which already partition the lattice into clusters. This includes density matrix renormalization group methods \cite{2} and Monte Carlo simulations using Hamiltonian partitioning \cite{3}.

Our letter is organized as follows. We begin by proving a general inequality involving two Hamiltonians which are equivalent within a projection subspace. We then apply the general inequality to a simple but illustrative example involving a one-dimensional periodic chain Hamiltonian and a non-periodic chain Hamiltonian. We then state and prove our main result, the lower energy bound. To conclude we check the lower bound numerically for our one-dimensional example and note the scaling of the error with cluster size.

After posting this preprint to the archive, it has come to our attention that the lower bound techniques presented here have already been discussed in the literature \cite{4}-\cite{6}.

2 General inequality

We prove a simple but useful result from which the lower energy bound follows as a special case. Let $H$ be a self-adjoint Hamiltonian. Let $P$ be a projection operator that projects onto a subspace $V_P$. We assume that $P$ commutes with $H$. Let $H'$ be any self-adjoint operator whose spectrum is bounded below and satisfies

$$PHP = PH'P.$$  \hfill (1)

Let $E'_0$ be the ground state energy of $H'$. For any vector $v$ we find

$$\langle Pv, HPv \rangle = \langle v, PHPv \rangle = \langle v, PH'Pv \rangle = \langle Pv, H'Pv \rangle.$$ \hfill (2)

Since

$$\langle Pv, H'Pv \rangle \geq E'_0 \langle Pv, Pv \rangle,$$ \hfill (3)

we conclude that

$$\langle Pv, HPv \rangle \geq E'_0 \langle Pv, Pv \rangle.$$ \hfill (4)

Therefore the spectrum of $H$ restricted to $V_P$ is bounded below by $E'_0$.

3 Application to lattice Hamiltonians

We now apply the general result \cite{1} to a translationally invariant lattice Hamiltonian. For clarity we consider a simple but sufficiently general example. Our example is a length $N$ one-dimensional periodic chain with one type of fermion. We define $O_1$ as a hopping term to and from the origin

$$O_1 = a_1^\dagger a_0 + a_0^\dagger a_1,$$ \hfill (5)
and $O_2$ as the number operator at the origin,

$$O_2 = a_0^\dagger a_0.$$  \hfill (6)

Our Hamiltonian describes a free one-dimensional fermion,

$$H = c_1 \sum_{n=0,...,N-1} \left[ a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1} \right] + c_2 \sum_{n=0,...,N-1} a_n^\dagger a_n.$$  \hfill (7)

Let us now take a four-site non-periodic chain and the renormalized Hamiltonian $H'$,

$$H' = \frac{c_3}{3} \sum_{n=0,1,2} T_n O_1 + \frac{c_4}{4} \sum_{n=0,1,2,3} T_n O_2.$$  \hfill (8)

The reason for the renormalization of coefficients will be apparent shortly. We define $E_0'$ as the ground state energy of $H'$ and take $P$ as the projection operator

$$P = \frac{1}{N} \sum_{n=0,...,N-1} T_n.$$  \hfill (9)

We note that

$$PH'P = \frac{c_3}{3} \cdot 3 \cdot PO_1 P + \frac{c_4}{4} \cdot 4 \cdot PO_2 P$$

$$= \frac{1}{N} PHP.$$  \hfill (10)

From (4) we conclude that the spectrum of $H$ in the translationally invariant subspace is bounded below by $N \cdot E_0'$.

## 4 Lower energy bound

We now state the general result, a lower energy bound for finite periodic lattices of any size or number of dimensions. Let $T_{\vec{r}}$ be the operator corresponding with translation by the vector $\vec{r}$. We observe that a local operator such as $a_{-\vec{r}}$ transforms as $T_{\vec{r}} a_{-\vec{r}} T_{-\vec{r}} = a_{-\vec{r}+\vec{r}}$. Let $G$ be any subgroup of lattice translations $T_{\vec{r}}$ and $|G|$ be the number of elements of $G$. Let $H$ be a lattice Hamiltonian defined by

$$H = \sum_{T_{\vec{r}} \in G} \left[ \sum_j c_j T_{\vec{r}} O_j T_{-\vec{r}} \right],$$  \hfill (11)

where the $c_j$’s are coefficients and $O_j$’s are general quantum operators. Let $H'$ be a modified Hamiltonian defined on a subset of lattice points,

$$H' = \sum_j \left[ \frac{c_j}{n_j} \sum_{k=1,...,n_j} T_{n_j,k} O_j T_{-n_j,k} \right].$$  \hfill (12)

The $n_j$’s are arbitrary positive integers and each $T_{n_j,k}$ is a lattice vector (not necessarily distinct). Let $E'_0$ be the ground state energy of $H'$. Since $H'$ and $\frac{1}{|G|} H$ are equivalent within the $G$-invariant subspace, we conclude from (4) that the energy spectrum of $H$ is bounded below by $|G| \cdot E'_0$. 

3
5 Numerical example

We now numerically check the lower energy bound for our one-dimensional chains. We use the notation $E_N^N(c_1, c_2)$ for the ground state energy of the periodic chain Hamiltonian in (5). This is trivially calculated in our example by momentum decomposition,

$$E_N^N(c_1, c_2) = \sum_{k=0, \ldots, N-1} \min(2c_1 \cos(\frac{2k\pi}{N}) + c_2, 0).$$

(13)

It easy to see that the lowest point of the spectrum in the translationally invariant subspace is also $E_N^N(c_1, c_2)$. We take $E_M^M(c_{M-1}, c_M)$ to be the ground state energy of the non-periodic chain Hamiltonian of length $M$. We have renormalized the coefficients as prescribed in (12). In Tables 1 and 2 we show $E_N^N(c_1, c_2)$ and the lower energy bound $N \cdot E_M^M(c_{M-1}, c_M)$ for several values of $N, M, c_1,$ and $c_2$. The values for $E_M^M(c_{M-1}, c_M)$ were calculated by Lanczos diagonalization.

Table 1. Lower bounds and energies for $c_1 = -1, c_2 = 0$

| $N$ | $N \cdot E_4^4$ | $N \cdot E_8^8$ | $N \cdot E_{12}^{12}$ | $N \cdot E_{16}^{16}$ | $E_0^N$ |
|-----|-----------------|-----------------|----------------------|----------------------|---------|
| 16  | -11.93          | -10.88          | -10.61               | -10.49               | -10.05  |
| 32  | -23.85          | -21.75          | -21.23               | -20.99               | -20.31  |
| 64  | -47.70          | -43.51          | -42.45               | -41.98               | -40.71  |
| 128 | -95.41          | -87.02          | -84.90               | -83.95               | -81.47  |

Table 2. Lower bounds and energies for $c_1 = -1, c_2 = 1$

| $N$ | $N \cdot E_4^4$ | $N \cdot E_8^8$ | $N \cdot E_{12}^{12}$ | $N \cdot E_{16}^{16}$ | $E_0^N$ |
|-----|-----------------|-----------------|----------------------|----------------------|---------|
| 16  | -4.63           | -4.08           | -3.90                | -3.76                | -3.53   |
| 32  | -9.26           | -8.17           | -7.79                | -7.52                | -7.00   |
| 64  | -18.52          | -16.33          | -15.59               | -15.05               | -13.96  |
| 128 | -37.04          | -32.67          | -31.18               | -30.10               | -27.91  |

We note that the error between the lower bound estimate and the actual energy scales as $M^{-1}$, the ratio of the boundary size to the bulk size of the cluster. This is also expected in the general case.

6 Summary

We have derived lower energy bounds for any translationally invariant lattice Hamiltonian. Our result is general and applies to virtually any local quantum lattice Hamiltonian relevant to particle, nuclear, or many-body physics. The lower bound is given in terms of the ground state energy for a renormalized Hamiltonian defined on a subset of lattice points. We find that the error scales as the ratio of the boundary size to the bulk size of the cluster. Given the simplicity, generality, and convenience of the result, we hope this lower bound estimate will be useful in many future computational lattice calculations.
References

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