Hubbard model on hypercubes

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Abstract

We present some exact results for the Hubbard model on $d$-dimensional hypercubes and fillings corresponding to $(N_{1/1} = N, N_{-1} = 1)$ with $N$ arbitrary. Introducing a spin formalism associated with the symmetry operations of the hypercube it is shown that the Hubbard model can be rewritten as a spin Hamiltonian defined on a $d \times (N + 1)$ rectangular spin lattice. For the two-electron case ($N = 1$) a logarithmic reduction of the active part of the Hilbert space can be achieved. It is shown that a very important size reduction can also be achieved for $N > 1$.

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The Hubbard model is one of the simplest many-body model used to describe strongly correlated fermions systems. Despite its formal simplicity, very little is known about the exact solution for $d$-dimensional lattices in the regime of intermediate dimensions $1 < d < \infty$, see, e.g., [1]. Here, we present some exact results for the Hubbard model on the $d$-dimensional hypercube $\gamma_d$ defined as the set of $N_s = 2^d$ sites whose $d$ coordinates are either 0 or 1. Hypercubes are related to usual cubic lattices with periodic boundary conditions: $\gamma_{2d}$ is topologically equivalent to a $d$-dimensional hypercubic lattice of linear size equal to 4 with periodic boundary conditions [2] (i.e., $\gamma_2$ is equivalent to the 4-sites ring, $\gamma_4$ equivalent to the two-dimensional $4 \times 4$ cluster with periodic conditions [3], etc.). In this paper we restrict ourselves to some specific fillings corresponding to an arbitrary number $N$ of electrons with a given spin (say $s_z = 1/2$) and only one single electron with opposite spin (say $s_z = -1/2$). The case $N = 1$ (two electrons with opposite spins) has been presented in detail in Ref. [2]. The main result was that a logarithmic reduction of the active part of the Hilbert space can be achieved. More precisely, the non-trivial ($U$-dependent) part of the spectrum can be expressed as the solution of a family of single-impurity problems defined on finite chains of size $d' + 1$ ($d' \leq d$). In other words, starting from the full initial Hamiltonian matrix of size $2^{2d}$ (two particles and $N_s = 2^d$ sites) we end up with a set of independent problems of size at most $d + 1$ (logarithmic reduction). Here, we extend this result to an arbitrary number $N$ of electrons with a given $s_z$-component and show that in some regime the logarithmic reduction is still valid.

We consider the standard Hubbard model with first-neighbor hopping term $t$ and on-site interaction energy $U$

\begin{equation}
H = -t \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_{i} c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow} = T(t) + V(U),
\end{equation}

for $(N + 1)$ electrons on $\gamma_d$. In contrast with our previous work [2] we introduce here a spin-formalism to express the action of the $d$ reflections $\pi_i$ of the full point symmetry group of the hypercube. To avoid confusion...
we distinguish with a label \( l \in \{1, \ldots, N\} \), each of the \( N \) spin-up particles, and denote the single spin-down electron with the label 0. We introduce relative positions for each particle \( l \in \{1, \ldots, N\} \) with respect to electron 0. Relative positions generate a new hypercube and can be labelled by an element of \( \{0, 1\}^d \), or \( \{\downarrow, \uparrow\}^d \) in a spin language. Accordingly, a state of the system is labelled by a configuration of a \( d \times (N + 1) \) rectangular spin lattice. A configuration for a given line defines a position on the hypercube. More precisely, the 0th line describes the position of the particle 0 whereas the line \( l \in \{1, \ldots, N\} \) describes the relative positions of particle \( l \). In this context we introduce \( |x\rangle^l_\alpha \), \( \alpha \in \{\downarrow, \uparrow\} \) as the \( \alpha \)th coordinate of the particle \( l \) on the hypercube \( (i \in \{1, \ldots, d\}, \ l \in \{0, \ldots, N\}) \). In terms of the Pauli matrix \( \sigma^\alpha_{l,i} \) defined at each site \( (i,l) \) of the spin lattice, the Hamiltonian can be written

\[
H = -t \sum_{i=1}^{d} \sigma^\uparrow_{l,i} \sigma^\downarrow_{l,i} - t \sum_{i=1}^{d} \sum_{l=0}^{N} \sigma^\uparrow_{l,i} + U \sum_{i=1}^{N} |\downarrow \cdots \downarrow\rangle \langle \downarrow \cdots \downarrow| .
\]

The motion of the reference particle 0 is not coupled to the rest of the system. Accordingly, the \( d \) operators \( \sigma^\alpha_{0,i} \) commute with \( H \). It follows that there are \( 2^d \) representations which can be labelled by a vector \((x^0_1, \ldots, x^0_d) \in \{-1, 1\}^d \) where \( x^0_0 \) is one of the two eigenvalues of \( \sigma^\alpha_{0,i} \). The Hamiltonian \( H \) being symmetric under the permutation of the columns, each representation depends only on the number of positive eigenvalues \( x^0_i \). For a given representation corresponding to \( p \) eigenvalues equal to one \( (p = 0, \ldots, d) \), the Hamiltonian reads

\[
H_p = -t \sum_{i=1}^{p} \sigma^\uparrow_{l,i} \sigma^\downarrow_{l,i} + t \sum_{i=p+1}^{d} \sigma^\downarrow_{l,i} \sigma^\uparrow_{l,i} - t \sum_{i=1}^{d} \sum_{l=0}^{N} \sigma^\uparrow_{l,i} + U \sum_{i=1}^{N} |\downarrow \cdots \downarrow\rangle \langle \downarrow \cdots \downarrow| .
\]

For the particular case \( N = 1 \), the Hamiltonian takes the simpler form

\[
H_p = -2t \sum_{i=1}^{p} \sigma^\uparrow_{l,i} + U |\downarrow \cdots \downarrow\rangle \langle \downarrow \cdots \downarrow| .
\]

The derivative of \( H \) is built as follows

\[
H_{S_p} = -2t \sum_{i=1}^{p} \sigma^\uparrow_{l,i} .
\]
important reduction of the size of the Hilbert space is obtained. In the favorable case \( N \ll d \), the reduction is logarithmic. Finally, let us mention that, in order to take into account the Pauli principle, eigenvectors need to be antisymmetrized with respect to the exchange of lines. This can be done by applying the corresponding fully antisymmetric projector.

References