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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 $(N_{\uparrow(\downarrow)} = N, N_{\downarrow(\uparrow)} = 1)$ 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 γ_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: γ_{2d} is topologically equivalent to a d-dimensional hypercubic lattice of linear size equal to 4 with periodic boundary conditions [2] (i.e., γ_2 is equivalent to the 4-sites ring, γ_4 equivalent to the two-dimensional 4×4 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 $d' + 1$ ($d' \leqslant d$). 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

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} c_{i\uparrow}^{+} c_{i\uparrow} c_{i\downarrow}^{+} c_{i\downarrow} = T(t) + V(U), \quad (1)$$

for $(N + 1)$ electrons on γ_d. In contrast with our previous work [2] we introduce here a spin-formalism to express the action of the d reflections π_i of the full point symmetry group of the hypercube. To avoid confusion

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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 $|\alpha\rangle_i^l$, $\alpha \in \{\downarrow, \uparrow\}$ as the ith coordinate of the particle l on the hypercube ($i \in \{1, \ldots, d\}$, $l \in \{0, \ldots, N\}$). In terms of the Pauli matrix $\sigma_{x,i}^l$ defined at each site (i,l) of the spin lattice, the Hamiltonian can be written

$$H = -t \sum_{i=1}^{d} \sigma_{x,i}^0 \sigma_{x,i}^1 \cdots \sigma_{x,i}^N - t \sum_{l=1}^{N} \sum_{i=1}^{d} \sigma_{x,i}^l + U \sum_{l=1}^{N} |\downarrow\downarrow \ldots \downarrow\rangle^{l\,l} \langle\downarrow\downarrow \ldots \downarrow|. \quad (2)$$

The motion of the reference particle 0 is not coupled to the rest of the system. Accordingly, the d operators $\sigma_{x,i}^0$ commute with H. It follows that there are 2^d representations which can be labelled by a vector $(\chi_1^0, \ldots, \chi_d^0) \in \{-1, 1\}^d$ where χ_i^0 is one of the two eigenvalues of $\sigma_{x,i}^0$. The Hamiltonian H being symmetric under the permutation of the columns, each representation depends only on the number of positive eigenvalues χ_i^0. For a given representation corresponding to p eigenvalues equal to one ($p = 0, \ldots, d$), the Hamiltonian reads

$$H_p = -t \sum_{i=1}^{p} \sigma_{x,i}^1 \cdots \sigma_{x,i}^N + t \sum_{i=p+1}^{d} \sigma_{x,i}^1 \cdots \sigma_{x,i}^N - t \sum_{l=1}^{N} \sum_{i=1}^{d} \sigma_{x,i}^l + U \sum_{l=1}^{N} |\downarrow\downarrow \ldots \downarrow\rangle^{l\,l} \langle\downarrow\downarrow \ldots \downarrow|. \quad (3)$$

For the particular case $N = 1$, the Hamiltonian takes the simpler form

$$H_p = -2t \sum_{i=1}^{p} \sigma_{x,i}^1 + U |\downarrow\downarrow \ldots \downarrow\rangle^{1\,1} \langle\downarrow\downarrow \ldots \downarrow|. \quad (4)$$

H_p is the sum of a free part and an impurity contribution expressed via a projection operator. In other words, the initial problem reduces to an effective one-electron problem (with a "renormalized" hopping term $-2t$) on a p-dimensional hypercube with an impurity at the origin. Let us denote by S_p the fully symmetric subspace (under permutation of the sites). Since the impurity term is non-zero only in S_p, the trivial (U-independent) part of the spectrum is obtained by considering the restriction of H to the orthogonal subspace $S_p^{\perp}$:

$$H_{S_p^{\perp}} = -2t \sum_{i=1}^{p} \sigma_{x,i}^1. \quad (5)$$

Now, in order to get the U-dependent part of the spectrum we introduce a set of $(p+1)$ properly symmetrized states $|l\rangle$ $(l = 0 \ldots p)$ spanning S_p. They are built as follows

$$|l\rangle = \frac{1}{\sqrt{p!\, l!\, (p-l)!}} \sum_{P \in S(p)} P |(\downarrow)^l, (\uparrow)^{p-l}\rangle, \quad (6)$$

where $S(p)$ denotes the permutation group for p objects. Using a second quantification formalism the Hamiltonian can be written

$$H_{S_p} = -2t \sum_{l=0}^{p} \sqrt{(p-l)(l+1)}\, a_{l+1}^{+} a_l + \text{h.c} + U a_0^{+} a_0. \quad (7)$$

This Hamiltonian describes a tight-binding model on a one-dimensional chain of length $p+1$ with an impurity site at the origin. Using the Koster–Slater approach [4] the one-particle Green's function can be calculated [2]. It can be shown that the eigenvalues of H_{S_p} satisfy the relation

$$\frac{1}{2^p} \sum_{l=0}^{p} \frac{\binom{p}{l}}{E + 2tp - 4tl} = \frac{1}{U}, \quad (8)$$

where $\binom{p}{l}$ is the binomial coefficient. This equation gives the non-trivial part of the spectrum.

In the two-electron case ($N = 1$) the logarithmic reduction of the size of the Hilbert space is possible because the spin Hamiltonian (4) is symmetric under the exchange of columns, i.e. all sites are equivalent. Such a symmetry property remains valid in the general case. More precisely, the general spin Hamiltonian (3) H_p is symmetric both under the set of permutations of the p first columns (denoted S_p^{+}) and the set of permutations of the $d-p$ last columns (denoted S_{d-p}^{-}). As a consequence, eigenvectors of H_p must be built within the different irreducible representations (IR) of the tensorial product $S_p^{+} \otimes S_{d-p}^{-}$. Derivation of RIs based on Young tableaux is quite technical and will be presented in detail elsewhere [5]. As a representative example, let us just consider the most symmetric RI obtained as the product of the two fully symmetric RIs of both groups. In this case, an arbitrary configuration of the spin lattice is entirely characterized by a set of positive integers $(n_1, \ldots, n_{2^N})$ with $\sum_{i=1}^{2^N} n_i = d$. Indeed, a column has only 2^N different configurations and the numbers n_i just give how many times a given configuration i appears in the full spin lattice configuration. As an important consequence, the size of the representation cannot exceed d^{2^N}. This result obtained for the most symmetric RI is in fact general [5]. Now, depending on the relative magnitude of N and d a more or less

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.

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