The Hubbard model on a complete graph: Exact Analytical results.

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Abstract

We derive the analytical expression of the ground state of the Hubbard model with unconstrained hopping at half filling and for arbitrary lattice sites.

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One of the most difficult problems in condensed matter physics is the characterization of the spectrum of strongly correlated Fermi systems. For 1-D integrable systems this can be done by Bethe ansatz. For non integrable systems or for higher dimensional ones, no generalizations of this method exist, the only resources being numerical methods. Exact diagonalizations of the Hubbard hamiltonian which take advantage of the conservation of the total number of electrons N , of the total spin in the z direction S_z as well as of the translational invariance of the lattice, has been performed by several authors [1, 2, 3]. In the case of the Hubbard model, however, one would like to use as basis functions the simultaneous eigenfunctions of S^2, S_z, N and of the operators characterizing the lattice. Basis functions which are invariant under $SU(2), U(1)$ and S_f (permutation group of f objects) can be easily constructed in terms of Young tableaux filled with quanta. By making projections on a particular subgroup of the permutation group S_f one could, in principle, construct proper basis functions for the Hubbard model on arbitrary lattices. In the present paper we consider the case of the Hubbard model on a complete graph (unconstrained hopping) and show how the above functions can lead to an analytical characterization of the ground state of the system valid for clusters of arbitrary sizes. In spite of the simplification introduced by the permutational symmetry, the model keeps all the complexity of the standard Hubbard model coming from the continuous symmetries and its solution may be useful for understanding the local properties of strongly correlated Fermi systems. Moreover, the lacking of exact analytical results for the Hubbard model in dimensions $D \neq 1$ makes the analytical solutions derived for this model a good test for numerical computations.
Let us start by introducing the Hubbard Hamiltonian on a complete graph

$$H = -t \sum_{\sigma i \neq j}^{f} c_{i_\sigma}^{\dagger} c_{j_\sigma} + U \sum_{i}^{f} n_{i_\uparrow} n_{i_\downarrow}. \tag{1}$$

where $c_{i_\sigma}^{\dagger}, c_{j_\sigma}$, (σ =$\uparrow$ or $\downarrow$) are standard fermionic creation and annihilation operators. The unconstrained hopping in Eq.(1) makes the system invariant under the action of the permutation group S_f. In addition to this discrete symmetry there are the known symmetries of the Hubbard model i.e. the $U(1)$ conservation of the total number of electrons $N = N_\uparrow + N_\downarrow = \sum_j \left(n_{j_\uparrow} + n_{j_\downarrow} \right)$, the $SU(2)$ invariance under rotations of the total spin $\vec{S}$ of the system, and the particle-hole symmetry. To define the Hilbert space of the states we denote with $|3>, |2>, |1>, |0>$, respectively, the doubly occupied state, the single occupied states with spin up and spin down, and the vacuum. The states of the system for a lattice of

f sites are products of single site states $|n_1 n_2 ... n_f >$ with $n_i \in \{0, 1, 2, 3\}$, the dimension of the Hilbert space being just 4^f. The conservation of the number operator allows to decompose the Hilbert space into a direct sum of eigenspaces corresponding to a fixed value of N. On the other hand, the invariance of the Hamiltonian under S_f allows to further block diagonalize this matrix with respect to the irreps of this group. Since the total spin of the system commutes with the permutation operator one can construct the irreps of $SU(2)$ in terms of Young tableaux filled with quanta. To this end it is convenient to introduce the quantum number

$$m = N + N_{\uparrow} \tag{2}$$

and consider all possible partitions $(m_1, m_2, ..., m_f)$ of m into f parts compatible with $N, N_{\uparrow}$, with $m_i = 0, 1, 2, 3$ and $m_1 \geq m_2 \geq ... \geq m_f$ (in eq. (2) we restrict to $N_{\uparrow} \geq N_{\downarrow}$ since the other cases follow from up-down symmetry). We remark that each partition is associated with an eigenstate $|m_1, m_2, ..., m_f >$ of S_z. This obviously leads to a family of states (eigenmanifolds of S_z) organized into levels. Each level of the hierarchy is characterized by a specific value of the number of "particles" m entering the states and by a specific value of $S_z = m - 3N/2$. From the above family of states one constructs eigenmanifolds of S^2, S_z with a given S_f symmetry by filling the quanta m_i, characterizing the states in each level, in the boxes of a Young tableau according to the following rules.
i) The quanta must be not increasing when moving from left to right in each row or when moving down each column of a given tableau.
ii) The quanta referring to spin up and spin down states ($m_i = 1, 2$) cannot appear more than once in a row.
iii) The quanta referring to doubly occupied states or to empty states ($m_i = 3, 0$) cannot appear more than once in a column.
These rules directly follow from the permutational properties of the states $|3 >, |2 >, |1 >, |0 >$ and from the symmetry property of Young tableaux. To characterize the eigenmanifolds of S^2, S_z with $S = S_z$ (highest spin vectors), one must identify the filled tableaux corresponding to the highest vectors of $SU(2)$. This can be done by noting that the application of the rising operator on a state associated to a given filled tableaux produces a state with the same S_f symmetry but with a 1 changed into a 2 (1-2 flip) i.e. a state associated to a tableaux of the $m + 1$ level. We have therefore, that the tableaux that satisfy the filling rules also after a 1-2 flip, are the ones for which $S > S_z$. It is worth to remark that by a $1 - 2$ flip two different m tableaux can be in general associated to the same $m + 1$ tableau. In this case one must take linear combinations $\phi_{\pm} = \psi_1 \pm \psi_2$ of the states corresponding to the m filled tableaux, to get one state with $S = S_z$ (ϕ_+) and one with $S = S_z + 1$

(ϕ_-). By construction, the basis functions so obtained are simultaneous eigenfunctions of N, S^2, S_z which span the irreps of S_f. With respect to these functions the hamiltonian matrix has a block diagonal form with the dimension of the blocks given by the number of "highest weight" tableaux one can fill with M quanta. The degeneracy of the corresponding eigenvalues is just $2S+1$ times the dimension of the corresponding S_f representation. We remark that the above set of rules can be easily implemented on a computer using symbolic programs like Mathematica [7]. We have used a Mathematica implementation of our method to study clusters of several sizes. From these studies the following conjecture about the ground state of the system can be made:

Conjecture: For $t, U > 0$ and for $N < 3$ the ground state of the system is always of symmetry type $\{f\}$. For $N \geq 3$ the symmetry of the ground state is of type $\{a_1, a_2, ..., a_r\}$ with r denoting the integer part of $(N+1)/2$, $a_1 = f - (N-2)$, $a_i = 2$ for $i = 2, ..., r-1$ and a_r equal to 2 or to 1 depending if N is even or odd. Furthermore, in the ground state S has always its minimal value ($S = 0$ for N even and $S = 1/2$ for N odd).

This conjecture appears natural since in the ground state one expects that the electrons will arrange (for $N < f$) in a configuration which minimizes the number of doubly occupied states and the tableaux listed above are just the ones which allow this. Using this conjecture we can easily derive analytical results for the ground state of the system. In particular, at half-filling and f even, the ground state is associated to an $S = 0$ ($m = \frac{3}{2}f$) tableau of type $\{2, 2, ..., 2\}$. From the filling rules it follows that there are only four possible ways of filling a tableau of this type with $\frac{3}{2}f$ quanta i.e. the ones reported in Fig.1. One easily check that only three of the states associated to these tableaux are $S = 0$ states. By denoting with $\psi_1, \psi_2, \psi_3, \psi_4$ the states associated with the tableaux from left to right of Fig. 1, we have that the states ψ_1, ψ_2 and $\psi_3 + \psi_4$ are $S = 0$ singlets (note that they are automatically orthogonal) while $\psi_3 - \psi_4$ is a $S = 1$ triplet. From the $S = 0$ states one can construct the 3×3 block characterizing the ground state of the system at half filling for arbitrary f as

$$\begin{pmatrix} 2\,U & t\sqrt{f(f/2-1)} & 0 \\ * & U & t\sqrt{f\,(f/2+1)} \\ * & * & 0 \end{pmatrix} \tag{3}$$

(the under diagonal elements were omitted since the matrix is symmetric), from which the ground state energy is readily obtained as

$$E_0 = U - \frac{(f^2\,t^2 + U^2)}{(3\,Z)^{\frac{1}{3}}} - \left(\frac{Z}{9}\right)^{\frac{1}{3}} \tag{4}$$

with

$$Z = 9\, f t^2 U - \sqrt{9\, f^2 t^2 U^2\, (9t^2 - f^2 t^2 - U^2) - 3\, (U^6 + f^6 t^6)}. \qquad (5)$$

We see that in both limits $U \to 0$ and $f \to \infty$, Eq.(4) reproduces the known expression $E_0 = -t\, f$ of the ground state energy [4]. Furthermore, the degeneracy of E_0 is just the dimension of the $\{2, 2, ..., 2\}$ representation i.e.

$$\frac{(f)!}{(\frac{f}{2}+1)!\frac{f}{2}!}. \qquad (6)$$

It is worth to note that although the lattice is not bipartite, the ground state at half filling is a singlet just as for bipartite lattices. This seems to indicate that this property is true for arbitrary lattices. We also remark that the above approach can be used to compute the ground state for arbitrary fillings. Thus, for example, for $N = 2$ the ground state energy is found by diagonalizing the $2 * 2$ matrix corresponding to the symmetric states with S=0, this giving

$$E_0 = 2\, t - f\, t + U/2 - (f^2 t^2 - 2tU + ftU + (U/2)^2)^{1/2}, \qquad (7)$$

while for $M = 3$ is obtained by diagonalizing the 3*3 block given by

$$\begin{pmatrix} U\, -\, (f/2-3)t & -t/2\sqrt{f(f-2)} & 1/2\sqrt{2\, f} \\ * & U\, -\, f/2 & -3\, t\sqrt{f/2-1} \\ * & * & -2(f\, -\, 3)t \end{pmatrix}. \qquad (8)$$

It is remarkable that for arbitrary fillings $N < f$ the ground state energy will always be obtained by diagonalizing a matrix of rank less or equal to four.

To check our result we have compared Eq.(4) with numerical diagonalizations of H up to clusters of 16 sites (this is the limit of computability on a supercomputer for this model). Thus, for example, for $f = 16$, $t = 1$, $U = 4$, one obtains with Lanczos method that the ground state energy is $E_0 = -12.719$ [5] while from Eq. (4) we get $E_0 = -12.7229$. The difference between these two values represents the error involved in the numerical computations at large values of f.

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Figure Captions Fig.1 Young tableaux of type $\{2, 2, ...\}$ filled with $M = \frac{3}{2}f$ quanta at $N = f$. The rectangular box represents $\frac{f}{2} - 2$ identical boxes.

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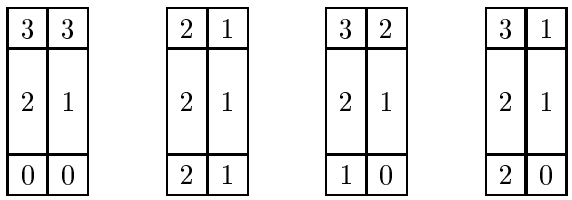
Fig.4