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Basis functions for strongly correlated Fermi systems

Mario Salerno

salerno@csied.dia.unisa.it *

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Abstract

A general method to construct basis functions for fermionic systems which account for the $SU(2)$ symmetry and for the translational invariance of the Hamiltonian is presented. The method does not depend on the dimensionality of the system and it appears as a natural generalization of the Bethe Ansatz to the case of non integrable systems. As an example we present the block diagonalization of the Hubbard hamiltonian for finite number of sites in one and two dimensions.

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*Department of Theoretical Physics, University of Salerno, 84100 Salerno, Italy.

During the past year a great deal of interest has been devoted to strongly correlated Fermi systems in two spatial dimensions because of their possible role as models for high T_c superconductivity [1]. Among these systems, the Hubbard model is certainly the simplest non trivial model for interacting electrons in a solid. Its Hamiltonian consists of a kinetic part, representing the electronic hopping between next neighbor sites and a a part representing the repulsive Coulumbian interaction of electrons with opposite spins on the same site. In spite of this apparent simplicity, the mathematical and the physical properties of this model in dimensions higher than one (magnetic properties of the ground state, existence of possible Mott transitions between insulating and conducting states, off-diagonal long range order, etc.), are still poorly understood. On the other hand, the large dimension of the Hilbert space of the states makes any numerical attempt to compute the spectrum of these systems possible only for clusters of very small size. A cluster of 6×6 lattice sites for the Hubbard model is already behind the computational power (using algorithms which account for the translational symmetry and for the conservation of the z component of the total spin S of the system), of any supercomputer nowadays available. The main difficulty is the lacking of general methods which allow to account for all the symmetries, both continuous and discrete, of these systems. For bosonic systems, basis functions which account for the conservation of the number operator and for the translational invariance on a periodic lattice can be constructed by the so called number state method [2]. In the case of the 2D Hubbard model one would like to use as basis functions the simultaneous eigenfunctions of S^2, of the total number electrons N and of the translational operator on the lattice. With respect to these functions the Hamiltonian would acquire a block diagonal form with blocks of minimal size (if all the symmetry is included), reducing in a significant manner the memory needed for the diagonalization procedure.

The aim of this letter is to present a general method to construct basis functions for strongly correlated Fermi systems which span the irreducible representations (irreps) of $SU(2), U(1)$, and of the translational group on a periodic lattice. The method does not depend on the dimensionality of the system and it appears to be a natural generalization of the Bethe Ansatz to the case of non integrable systems (in the case of the one-dimensional antiferromagnetic Heisenberg chain it is completely equivalent to Bethe Ansatz). The method is based on the following points: i) The invariance of the total spin of the system under the permutation group S_f allows to construct basis functions which span the irreps of $SU(2)$. This is done by using "filled" Young tableaux for fermionic systems recently introduced in ref. [3]. ii) Any discrete group is a subgroup of the permutation group, thus one can project the above eigenfunctions on the S_f subgroup of interest (in the present case on the subgroup corresponding to the translations on the lattice). The commutation of the translation operator with the total spin S, assures that the projected functions will be simultaneous eigenfunctions of both operators. We illustrate the method by taking as working example the Hubbard model both in one and in two dimensions.

The Hubbard Hamiltonian is written as

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

As usual, U represents the onsite Coulomb repulsion energy between electrons, $n_{i_\uparrow}$ and $n_{i_\downarrow}$ are respectively, spin up and spin down occupation number operators at site i, t denotes the hopping energy between sites, σ denotes the possible spin states of the electrons (i.e. $\sigma =\uparrow$

or $\downarrow$), and $c^{\dagger}_{i_\sigma}, c_{j_\sigma}$ are fermionic creation and annihilation operators

$$\{c_{i_\sigma}, c_{j_{\sigma'}}\} = \left\{c\dagger_{i_\sigma}, c^{\dagger}_{j_{\sigma'}}\right\} = 0, \quad \left\{c_{i_\sigma}, c^{\dagger}_{j_{\sigma'}}\right\} = \delta_{i,j}\delta_{\sigma,\sigma'}. \tag{2}$$

As well known the Hamiltonian (1) posses, besides the translational symmetry and the SU(2) invariance under rotations of the total spin $\vec{S}$ of the system, also the $U(1)$ conservation of the total number of electrons

$$N = \sum_j \left(n_{j_\uparrow} + n_{j_\downarrow}\right), \tag{3}$$

and the so called particle-hole symmetry. The conservation of N and S_z obviously implies the separate conservation of the number of electrons with spin up $N_\uparrow = \sum_j n_{j_\uparrow}$ and of electrons with spin down $N_\downarrow = \sum_j n_{j_\downarrow}$. To define the Hilbert space of the states we denote with $|3>, |2>, |1>, |0>$ the possible states on a generic site i.e., respectively, the doubly occupied state, the single occupied state with spin up, the single occupied state with spin down and the vacuum (the numbers 3,2,1,0 are here used as quantum numbers to characterize them). Since there are four possible states at each site, the dimension of the Hilbert space for a lattice with f sites is just 4^f. On the other hand the conservation of the number operator N allows to decompose the Hilbert space K into a direct sum of eigenspaces K_N corresponding to a fixed value of N. The dimension of these spaces is just the number of ways N electrons can be placed in $2f$ boxes i.e. $d_N = \frac{(2f)!}{(2f-N)!N!}$. This leads to the diagonalization (for each N) of a finite $d_N \times d_N$ matrix (we can restrict N to $N \leq f$ since $f < N \leq 2f$ follows from the particle-hole symmetry). We then use the invariance of S^2 under S_f to construct S^2, N eigenfunctions which allow to further block diagonalize each $d_N \times d_N$ matrix with respect to the irreps of $SU(2)$. To this end we recall that the irreducible representations of S_f can be labelled by all possible partitions $[f_1 ... f_k]$ of f into k parts, with f_i integers obeying $f_1 \geq f_2 \geq ... \geq f_k$ and $f_1 + f_2 + ... + f_k = f$. To each partition it is associated a Young tableau of type $\{f_1, f_2, ...\}$ i.e. having f_1 boxes in the first row, f_2 boxes in the second row, etc., each tableau corresponding to different symmetry class operations of S_f [4].

In order to obtain the highest weight vectors of $SU(2)$ (i.e. eigenvectors of S^2, S_z belonging to $S = S_z$) with a given S_f symmetry we use the idea of Young tableaux "filled" with quanta, introduced for bosonic systems in ref. [5] and extended to the fermionic case in ref. [3]. To this end we observe that for a fixed $N = N_\uparrow + N_\downarrow$, the possible values of $N_\uparrow, N_\downarrow$ compatible with it are all the partitions of N into two parts, each partition being associated with a well defined value of S_z. Let us introduce the quantum number

$$M = 3N_\downarrow + 2(N_\uparrow - N_\downarrow) \tag{4}$$

and consider all the partitions $(m_1, m_2, ..., m_f)$ of M into f parts with $m_i = 0, 1, 2, 3$ (in eq. (4) and in the following, we restrict to $N_\uparrow \geq N_\downarrow$ since the cases $N_\uparrow < N_\downarrow$ follows from these by interchanging spin up with spin down electrons). Since the order of the quantum numbers m_i in the partition is unimportant we fix it to be $m_1 \geq m_2 \geq ... \geq m_f$. We remark that each partition $(m_1, m_2, ..., m_f)$ of M is associated with an eigenstate $|m_1, m_2, ..., m_f>$ of S_z. This leads to a family of states organized into levels. From each M level we construct eigenmanifolds of S^2 with a given S_f symmetry by filling the quanta m_i, characterizing that 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 (i.e. $m_i = 1, 2$) cannot appear more than once in a row. iii) The quanta referring to doubly occupied states or to empty states (i.e. $m_i = 3, 0$) cannot appear more than once in a column. These rules directly follow from the permutational properties of the four states $|3>, |2>, |1>, |0>$ and from the symmetrization and antisymmetrization property of, respectively, rows and columns of a given Young tableau. By using these rules we construct, for each M level, a family of filled Young tableaux for each S_f symmetry. To pass from filled tableaux to states we apply Young symmetrizer and antisymmetrizer operators which take into account the Pauli exclusion principle, i.e. every time the symmetry operator involves the permutation of n_a spin up electrons and n_b spin down electrons an extra $(-1)^{n_a+n_b}$ factor is included (note that due to the permutational properties of the $|2>$ and $|1>$ states, one must count only the interchanges of spin electrons and spin down electrons separately involved in each permutation). These states, by construction, are eigenstates of S_z with a given S_f symmetry but, in general, they are not eigenstates of S^2. In order to identify the M levels with the eigenmanifolds of S^2 we must characterize the filled tableaux corresponding to highest vectors of $SU(2)$ (highest weight filled tableaux). This can be done by noting that a change of a 1 into a 2 (1-2 flip) in a filled tableau corresponds to increases M by 1 i.e. to pass to a filled tableau of the $M+1$ level. We have therefore, that the filled tableaux which survive 1-2 flips (i.e. the one that satisfy the filling rules also after a 1-2 flip) are the ones for which $S > S_z$. In this way one "extract" from each M level the highest weight vectors of SU(2). We remark, however, that by a $1-2$ flip two different M tableaux may be associated with the same $M+1$ tableau. In this case one can prove that the linear combinations $\phi_\pm = \psi_1 \pm \psi_2$ of the states corresponding to the M filled tableaux, produce one $S = S_z$ state (ϕ_+) and one $S = S_z + 1$ state (ϕ_-). Note that these states are not necessarily orthogonal so that, in general, a final Gram-Schmidt orthonormalized procedure must be applied. We remark that the functions so constructed are good basis functions to solve fermionic systems with infinite-range interactions (in the thermodynamic limit this should correspond to exact mean-field calculations). The application of these functions to the Hubbard model with unconstrained hopping is discussed in ref. [3]. By using these functions one can easily get the following characterization of the ground state for the S_f-invariant Hubbard system for $t > 0$: the N=1,2 ground state is always associated with a tableau of type $\{f\}$ while for $f \geq 3$ it is associated with tableau of type $\{f-(N-2), 2, ..., 2\}$ for N even or of type $\{f-(N-2), 2, ..., 2, 1\}$ for N odd. Furthermore, in the ground state S has always its minimal value i.e. $S = 0$ for N even or $S = \frac{1}{2}$ for N odd.

We now come to the problem of projecting the above functions on the subgroup, say G, of S_f of physical interest (for translations on a 1D periodic lattices G is just the abelian group C_f corresponding to the cyclic permutations). This problem is similar to the one encountered in perturbation theory when a perturbation reducing the symmetry induces a splitting in the energy levels. Let us denote by $D(R), R \in S_f$ the irreps of S_f. A representation of G is readily obtained by selecting among the matrices $D(R)$ those corresponding to elements of G. These representations however are in general reducible i.e. they can be expressed in terms of irreps $D^{(\nu)}$ of G as $D(R) = \sum_\nu c_\nu D^{(\nu)}(R)$ with c_ν non negative integers counting the number of times $D^{(\nu)}$ appears in D. By denoting with g_i the number of elements in the class K_i of G and with g the order of this group, one easily express the integers c_ν in terms

of the characters $\chi, \chi^{(\nu)}$ of respectively S_f and G as

$$c_\nu = \frac{1}{g} \sum_i g_i \chi_i^{(\nu)\,*} \chi_i. \tag{5}$$

This gives the splitting of the irreps of S_f (i.e. of the Young tableaux of a given type) into the irreps of G (star in Eq.(5) denotes complex conjugation). The eigenfunctions ψ of N, S^2, corresponding to the above highest weight filled Young tableaux, are projected on the $\nu-$th irrep of G by using the projection operator $P^{(\nu)}$ defined by

$$\psi^{(\nu)} = P^{(\nu)}\psi \equiv \frac{n_\nu}{g} \sum_R \chi^{(\nu)\,*}(R)\ U_R \cdot \psi \tag{6}$$

where the sum is over all the elements R of the S_f subgroup, n_ν is the dimension of the ν-th irrep of G, $\chi^{(\nu)}(R)$ the corresponding characters and U_R the operator associated to the group element R [4]. By taking G to be the subgroup corresponding to the lattice translations T_n and by projecting all the functions corresponding to highest weight filled Young tableaux with a given value of S and N, we get the simultaneous eigenfunctions of N, S^2, T_n with respect to which the Hamiltonian aquires block diagonal form.
Let us illustrate the method with an explicit calculation on the Hubbard model with $f = 4$. We consider the four sites disposed in two different configurations: the first corresponding to a 1-D periodic chain, the second to a 2-D periodic square lattice. In the first case the S_f subgroup of interest is the cyclic group C_4, while in the second case is the group C_{2h}. They are both abelian groups with one dimensional irreps. Let us denote with A, B, E_1, E_2, the irrep of C_4 and with A_u, A_g, B_u, B_g the irrep of C_{2h} (we refer to the standard notation of point-symmetry groups). The two irrep E_1, E_2 of the group C_4 are one the complex conjugate of the other thus they physically correspond to a double degenerate level (this is true also for other C_f groups). This accidental degeneracy is connected to time reversal invariance of the Hubbard Hamiltonian i.e. the complex conjugate of an eigenfunction is automatically an eigenfunction with the same energy. We take advantage of this fact by considering E_1, E_2 equivalent to a single irrep E of dimension two. For brevity we concentrate only on the case $S = 0$ at half filling ($N = 4$) (a detailed analysis will be published elsewhere [6]). In Table 1 we report all the $S = 0$ highest weight filled tableaux together with their splittings in terms of the irreps of the groups C_4, and C_{2h}. From this table we see that for the 1-D chain one gets two blocks of dimension 6×6 associated with the irrep A and B (this giving 12 $S = 0$ nondegenerate eigenvalues), and one 4×4 block associated to the irrep E (giving four doubly degenerate eigenvalues). In the case of the 2D chain we see that the accidental degeneracy in the E representation is removed, and we have three 4×4 blocks (respectively associated to the irreps A_u, B_u, B_g) and one 8×8 block associated to the A_g representation. Let us concentrate here only on the ground state. To this end we remark that for the S_f-invariant Hubbard system the ground state is characterized by a $S = 0$ Young Tableau of type $\{2, 2\}$ (see above discussion and ref. [3] for details). We conjecture that the projection on the translational subgroup will not alter this situation, i.e. that the ground state belongs to one of the irrep in which the S_f ground state splits (we think this conjecture holds true for general cases if f is even and $t > 0$). This is indeed what happens for the present cases. We find that the ground state is of type B for the 1-D chain and of type A_g for the 2-D chain.

The block associated to the B representation of the 1D chain is given by

$$\begin{pmatrix} 2\,U & \frac{-4\,t}{\sqrt{3}} & -\left(\sqrt{\frac{8}{3}}\,t\right) & 0 & 0 & 0 \\ \frac{-4\,t}{\sqrt{3}} & \frac{8\,t}{3}+U & \frac{-\left(2^{\frac{3}{2}}\,t\right)}{3} & 0 & 0 & 0 \\ -\left(\sqrt{\frac{8}{3}}\,t\right) & \frac{-\left(2^{\frac{3}{2}}\,t\right)}{3} & \frac{-8\,t}{3}+U & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\,U & 0 & -2\,t \\ 0 & 0 & 0 & 0 & 0 & 2\sqrt{3}\,t \\ 0 & 0 & 0 & -2\,t & 2\sqrt{3}\,t & U \end{pmatrix}, \tag{7}$$

while the block associated to the A_g representation of the 2D chain is:

$$\begin{pmatrix} 2\,U & \frac{-16\,t}{3} & 0 & 0 & \sqrt{\frac{32}{3}}\,t & 0 & 0 & \frac{2^{\frac{5}{2}}\,t}{3} \\ \frac{-16\,t}{3} & U & \frac{-\left(2^{\frac{3}{2}}\,t\right)}{3} & \sqrt{\frac{8}{3}}\,t & 0 & \sqrt{\frac{8}{3}}\,t & -\left(2^{\frac{3}{2}}\,t\right) & 0 \\ 0 & \frac{-\left(2^{\frac{3}{2}}\,t\right)}{3} & 2\,U & 0 & \frac{4\,t}{\sqrt{3}} & 0 & 0 & \frac{-8\,t}{3} \\ 0 & \sqrt{\frac{8}{3}}\,t & 0 & 0 & -4\,t & 0 & 0 & \frac{8\,t}{\sqrt{3}} \\ \sqrt{\frac{32}{3}}\,t & 0 & \frac{4\,t}{\sqrt{3}} & -4\,t & U & 0 & 0 & 0 \\ 0 & \sqrt{\frac{8}{3}}\,t & 0 & 0 & 0 & 2\,U & 0 & \frac{-4\,t}{\sqrt{3}} \\ 0 & -\left(2^{\frac{3}{2}}\,t\right) & 0 & 0 & 0 & 0 & 0 & 4\,t \\ \frac{2^{\frac{5}{2}}\,t}{3} & 0 & \frac{-8\,t}{3} & \frac{8\,t}{\sqrt{3}} & 0 & \frac{-4\,t}{\sqrt{3}} & 4\,t & U \end{pmatrix}. \tag{8}$$

To check these results we have numerically diagonalized H in both cases in the $N = 4$ eigenspace of dimension $d_4 = 70$. From these calculations it follows that, for $t = 1, U = 2$ and for $f = N = 4$, the ground state of the 1D chain is non degenerate with energy $E = -2.82843$ while for the 2D chain the ground state is non degenerate with energy $E = -6.681695$. One easily verify that these values coincide with those obtained by diagonalizing the blocks respectively in Eq.(7) and Eq.(8).

In closing this letter we remark that the above method of block diagonalizing H is quite general and can be applied to more complicate fermionic systems such as the Anderson model as well as to other subgroups (besides translations) of physical interest such as the invariance group of fullerene molecules. Furthermore we note that the study of the Heisenberg model and of the t-J model in one and two dimensions directly follow from the above analysis by restricting the space of the single site states respectively to $|0>, |1>$ (Heisenberg) or $|0>, |1>, |2>$ (t-J). We also remark that the method is completely algebraic and can be easily implemented on a computer (by using Mathematica [7] we have set up packages which performs all the operations to construct the above basis functions). We hope our method will facilitate future numerical studies of strongly correlated Fermi systems contributing to the understanding of the physical properties of these systems in two and three dimensions.

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Table Captions

Table 1

Decomposition of the filled Young tableaux corresponding to $S = 0$ highest weight vectors of $SU(2)$ for $f = N = 4$, in terms of the irrep of the groups C_4, and C_{2h}. The sum of tableaux denotes the (plus) linear combination of the corresponding states.

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S_4	C_4	C_{2h}
$\begin{array}{\|c\|c\|c\|c\|}\hline 3 & 3 & 0 & 0 \\ \hline \end{array}$	A	A_g
$\begin{array}{\|c\|c\|c\|c\|}\hline 3 & 2 & 1 & 0 \\ \hline \end{array}$	A	A_g
$\begin{array}{\|c\|c\|c\|}\hline 3 & 3 & 0 \\ \hline \end{array}$ $\begin{array}{\|c\|}\hline 0 \\ \hline \end{array}$	$B\,,E$	$A_u\,,B_u\,,B_g$
$\begin{array}{\|c\|c\|c\|}\hline 3 & 2 & 1 \\ \hline \end{array}$ $\begin{array}{\|c\|}\hline 0 \\ \hline \end{array}$	$B\,,E$	$A_u\,,B_u\,,B_g$
$\left(\begin{array}{\|c\|c\|c\|}\hline 3 & 2 & 0 \\ \hline \end{array} \begin{array}{\|c\|}\hline 1 \\ \hline \end{array} + \begin{array}{\|c\|c\|c\|}\hline 3 & 1 & 0 \\ \hline \end{array} \begin{array}{\|c\|}\hline 2 \\ \hline \end{array} \right)$	$B\,,E$	$A_u\,,B_u\,,B_g$
$\begin{array}{\|c\|c\|}\hline 3 & 3 \\ \hline \end{array}$ $\begin{array}{\|c\|c\|}\hline 0 & 0 \\ \hline \end{array}$	$A\,,B$	$A_g\,,A_g$
$\begin{array}{\|c\|c\|}\hline 2 & 1 \\ \hline \end{array}$ $\begin{array}{\|c\|c\|}\hline 2 & 1 \\ \hline \end{array}$	$A\,,B$	$A_g\,,A_g$
$\left(\begin{array}{\|c\|c\|}\hline 3 & 2 \\ \hline \end{array} \begin{array}{\|c\|c\|}\hline 1 & 0 \\ \hline \end{array} + \begin{array}{\|c\|c\|}\hline 3 & 1 \\ \hline \end{array} \begin{array}{\|c\|c\|}\hline 2 & 0 \\ \hline \end{array} \right)$	$A\,,B$	$A_g\,,A_g$
$\left(\begin{array}{\|c\|c\|}\hline 3 & 2 \\ \hline \end{array} \begin{array}{\|c\|}\hline 1 \\ \hline \end{array} \begin{array}{\|c\|}\hline 0 \\ \hline \end{array} + \begin{array}{\|c\|c\|}\hline 3 & 1 \\ \hline \end{array} \begin{array}{\|c\|}\hline 2 \\ \hline \end{array} \begin{array}{\|c\|}\hline 0 \\ \hline \end{array} \right)$	$B\,,E$	$A_u\,,B_u\,,B_g$