SO(4) invariant basis functions for strongly correlated Fermi systems

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Abstract

We show how to construct SO(4) invariant functions for strongly correlated Fermi systems on lattices of finite sizes. We illustrate the method on the case of the 1D Hubbard chain with four and with six sites.

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During the past years a great deal of interest has been devoted to the study of strongly correlated Fermi systems because of their possible role as models of high $T_c$ superconductivity\cite{1}. Among these systems, the Hubbard model is certainly the simplest non trivial model for interacting electrons in a solid. In spite of its apparent simplicity, the mathematical and physical properties of this model, in dimensions higher than one, are still poorly understood. On the other hand, the huge dimension of the Hilbert space ($4^f$ for a lattice of $f$ sites) severely restricts numerical studies to clusters of small sizes. In order to reduce the dimension of this space one may use the symmetry properties of the Hamiltonian. Basis functions which account for the conservation of the number operator, for the conservation of the $z$ component of the total spin $S$ and for the translational invariance, were constructed by many authors\cite{2,3}. For the Hubbard model on bipartite lattices, however, one would like to use as basis functions the simultaneous eigenfunctions of the $SO(4)$ (spin $S$ and pseudospin $J$) algebra as well as of the translation operator.

The aim of the present paper is to show how to construct $SO(4)$ invariant functions for strongly correlated Fermi systems on arbitrary lattices. As a result we give a set of rules for constructing such functions which are easy to implement on a computer in terms of symbolic languages. We illustrate the method on the example of the Hubbard chain with $f = 4$ and $f = 6$ sites. For $f = 4$ we find that the $SO(4)$ diagonalization decomposes the original $256 \times 256$ hamiltonian matrix into blocks of dimension less or equal to four. The ground state at half filling is obtained by diagonalizing a $3 \times 3$ block corresponding to $S = J = 0$ and with momentum equal to $k = \pi$. In the case of the $f = 6$ chain we find that the ground state at half filling is obtained by diagonalizing a $14 \times 14$ band matrix corresponding to the $S = 0, J = 0, k = \pi$ space, with the width of the band equal to six. Finally, at the end of the paper, we estimate the sizes of the $SO(4)$ blocks as a function of $f, J, S$.

Let us start by introducing the Hubbard Hamiltonian as

$$H = -t \sum_{\sigma \tau} c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma} + U \sum_i n_i \cdot n_i,$$  \hspace{0.5cm} (1)

where $c_{i,\sigma}^\dagger$, $c_{i,\sigma}$, ($\sigma = \uparrow$ or $\downarrow$), are usual fermion creation and annihilation operators. As well known, this model is invariant under $SU(2)$ spin rotations with generators

$$S^+ = \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}, \quad S^- = (S^+)^\dagger, \quad S_z = \frac{1}{2}(N_\uparrow - N_\downarrow).$$  \hspace{0.5cm} (2)

and under $SU(2)$ pseudo-spin rotations with generator

$$J^+ = \sum_i (-1)^i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger, \quad J^- = \sum_i (-1)^i c_{i,\downarrow} c_{i,\uparrow}, \quad J_z = \frac{N - f}{2}.$$  \hspace{0.5cm} (3)

One readily checks that $S, S_z, J, J_z, H$ form a complete set of computable observables. Moreover, from the expression of $S_z, J_z$ in Eq.s (2,3) it is evident that the states of the system must have spin and pseudospin both integer or both half integer, this giving a $Z_2$ reduction which leads to a global $SO(4)$ symmetry\cite{4}. To construct the basis functions which span the irreducible representations of $SO(4)$ we will use the representation theory of the permutation group. As well known, Young tableaux are natural objects for this purpose. To this end we remark that the commutation between the permutation operations and the spin rotations implies that the irreps of $S_f$ are automatically irreps of the $SU(2)$ spin algebra. This was used in ref.\cite{5,6} to solve the
Hubbard model with unconstrained hopping for clusters of arbitrary sizes. Here we extend this result to the $SO(4)$ symmetry and to arbitrary lattices. To this end let us denote with the symbols $|3\rangle,|2\rangle,|1\rangle,|0\rangle$ the four states on a given site (respectively the doubly occupied, the single occupied spin up and spin down states and the vacuum) and let us introduce the quantum number

$$M = \frac{3}{2}(f - 2J_z) + S_z. \quad (4)$$

Eigenmanifolds of $S^2, S_z, J^2, J_z$ can be constructed from the irreps of $S_f$ by considering all possible partitions $(m_1, m_2, ..., m_f)$ of $M$ into $f$ parts (compatible with $N, S_z, J_z$), with $m_i = 0, 1, 2, 3, m_1 \geq m_2 \geq ... \geq m_f$, and by filling the quanta $m_i$ of each partition in the boxes of a Young tableaux according to the following rules.

i) The quanta must not increase when moving from left to right in a row or when moving down in a column.

ii) The quanta referring to spin up and spin down states ($m = 1, 2$) must not appear more than once in a row.

iii) The quanta referring to doubly occupied states or to empty states ($m = 3, 0$) must not appear more than once in a column.

To pass from Young tableaux to states one usually apply standard Young symmetrizer and antisymmetrizer operators $[7]$. Here, however, due to the fermion realization of the spin algebra, one must include minus signs in the permutations which involve the interchange of two fermions to account for the Pauli exclusion principle. Moreover, an additional $(-1)^g$ sign is required for the permutations which involve doubly occupied states at site $j$ to balance the alternating sign of the pseudospin algebra (without this sign the states would be eigenstates of $S, S_z, J_z$, but not necessarily of $J$). To select among the filled Young tableaux the ones corresponding to highest weight vectors of $SO(4)$, (actually highest weights for spin and lowest weights for pseudospin) we use the following criterion. Let us call the change of a spin down into a spin up a $1-2$ flip and the change of a double occupied state into an empty state a $3-0$ shift. We note that $S^+$ just performs $1-2$ flips while $J^-$ performs $3-0$ shifts. It is clear that the filled tableaux which become inconsistent with the filling rules after $1-2$ flips and $3-0$ shifts are annihilated by both $S^+$ and $J^-$ i.e. they are highest-lowest weight vectors of the $SO(4)$ algebra. On filled tableaux then, we perform $1-2$ flips (i.e. turn a $1$ into a $2$ in all possible manners) to select the highest weights vectors of the spin $SU(2)$, and $3-0$ shifts to select the lowest weights of the pseudospin algebra. Note that according to our rules, double occupied states must be in the first row of a tableaux in consecutive order from the first box on the left. One can shift out a double occupied state of the first row without changing the spin symmetries, by moving the quanta one unit to the left and inserting a zero in the end box of the row, or by moving the quanta in the first column one unit upward and inserting a zero in the end box of the column. The tableaux that become inconsistent with the filling rules under both $1-2$ flips and $3-0$ shiftings are the highest-lowest weight vectors of the $SO(4)$ algebra. We remark however, that by $1-2$ flips and $3-0$ shifts two different tableaux can be related to the same tableau of higher (lower) spin (pseudospin). In this case, linear combinations of the corresponding states must be taken. Having constructed the $SO(4)$ invariant states we come to the problem of projecting them on a particular subgroup, say $G$, of $S_f$ (we recall that any discrete group is a subgroup of $S_f$). To this end we 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 $c_\nu$ 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 $c_\nu$ in terms of the characters $\chi, \chi^{(\nu)}$ of respectively $S_f$ and $G$ as

$$c_\nu = \frac{1}{g} \sum_i g_i \chi^{(\nu)}_i \chi_i.$$  \hfill (5)

This gives the splitting of the irreps of $S_f$ into the irreps of $G$ (here $*$ denotes complex conjugation). The eigenfunctions $\psi$ of $S^2, J^2$, corresponding to the above highest-lowest weight states, are then projected on the $\nu$-th irrep of $G$ by using the projection operator $P^{(\nu)}$,

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

where the sum is over all the elements $R$ of the $S_f$ subgroup ($n_\nu$ is the dimension of the $\nu$-th irrep of $G$, $\chi^{(\nu)}_R (R)$ the corresponding characters and $U_R$ the operator associated to the group element $R$). By taking $G$ to be the subgroup corresponding to the lattice translations $T_n$ we get the simultaneous eigenfunctions of $S^2, J^2, T_n$ with respect to which the Hamiltonian acquires a block diagonal form. To illustrate the method let us consider the case of the Hubbard model on a 1D periodic chain with $f = 4$. This case corresponds to take the cyclic subgroup $C_4$, of $S_4$ which is an abelian group with 1D irreps denoted by $A, B, E_1, E_2$. The irreps $E_1, E_2$ are one the complex conjugate of the other thus they are associated to the same energy level. We can take advantage of this accidental degeneracy by considering $E_1, E_2$ equivalent to a single irrep $E$ of dimension two (note that this degeneracy is connected with the time reversal invariance of the Hubbard hamiltonian). In Table 1 we have reported the filled tableaux associated to the highest-lowest weight vectors of the spin and pseudo-spin algebra constructed with our rules, for even values of the fillings (the odds fillings follow similarly and will be omitted for brevity). In this table we have also reported the splitting of the tableaux under the translation group. Note that, due to the presence of the $(-1)^j$ sign in the Young operators, the even and odd representations of $C_4$ are interchanged in the tableaux containing odd numbers of double occupied states.

From Table 1 we see that the $N=0$ sector contains only one state (the vacuum) with eigenvalue $E_0 = 0$. This state is a singlet under $S$ and a quintet under $J$. The application of the pseudospin rising operator to it, generates an eigenstate of $H$ of the $N=2$ sector with $S = 0, J = 2$ but with $J_z = 1$. The corresponding eigenvalue is $E_2 = U$ (the state does not appear in our table since it is not a lowest weight). By further applications of $J^+$ to the vacuum on gets all its descendents to higher (even) fillings

$$E_N = E_0 + \frac{N}{2} U, \quad N = 2, 4, ..., 2f.$$  \hfill (7)

This is a general feature of the $SO(4)$ diagonalization i.e. with the rising operator $J^+$ we can map all the spectrum computed at lower fillings $N$ to the higher fillings $N + 2n, \quad n = 1, 2, ..., f - N/2$.

From Table 1 we also see that the $N = 2, S = 1$ sector decomposes into two $1 \times 1$ blocks (A, B states) and one $2 \times 2$ block (E states) for a total of 18 states, while the $N = 2, S = 0$ sector decomposes into three blocks, two are $2 \times 2$ (B, E states) and one is $3 \times 3$ (A states) for a total of 9 states. The dimension of the $N = 2$ sector is then $18 + 9 + 1 = 28$ (note the addition of the state $J = 2, J_z = 1$, coming from the $N = 0$ sector). Similarly we see that the $N = 4$ sector contains 10 states with $S = 0, 9$ states with $S = 1$ and one state with $S = 2$, for a total of 42 states. If one adds these states to the ones coming from lower (even) fillings one gets the total dimension of the $N = 4$ sector as $42 + 18 + 9 + 1 = 70$. These numbers just coincide with the ones obtained from the usual formula $d_N = \binom{2f}{N}$ for $N$ electrons on 2f sites. By rising these states to higher
fillings we get the total dimension of the Hilbert subspace corresponding to the even fillings as $1 \times 5 + 27 \times 3 + 42 = 128$. One checks that this number is just the sum of all the tableaux in Table 1 taken with their multiplicities (i.e. the product of the tableaux dimension times the spin and pseudospin degeneracies). This checks the completeness of our basis (the same analysis performed on odd fillings gives others 128 eigenvalues for a total of $4^4$ states). In Tables 2a, 2b we have reported the $SO(4)$ block decomposition of the hamiltonian matrix corresponding to the states listed in Table 1. Note that the eigenvalues at higher (even) fillings are obtained by diagonalizing the same blocks of Tables 2 but with an $U$ added to the diagonal elements for each application of $J^+$ (the blocks at half filling obviously do not have descendents since $J = 0$). As expected, the ground state at half filling is a singlet with $S = J = 0$ [8]. It is of interest to note that this state has momentum $k = \pi$ (B state) and comes from the splitting of the same tableaux which characterizes the ground state of the $S_f$ invariant Hubbard model (see [3, 8]). One can easily compare these results with direct numerical diagonalizations in the full Hilbert space. Thus, for example, for $N = 4$ ($d_4 = 70$) one finds that at $t = .75, U = 1.5$ the ground state is a singlet with energy $E = -2.12132$. This is just the same value obtained from the $S = J = 0, B$ block of Table 2a.

Using the $SO(4)$ symmetry we have also investigated a chain with $f = 6$ sites. Here for brevity we report only on the ground state at half filling (more details will be given elsewhere). In this case we find that the ground state is obtained by diagonalizing a $14 \times 14$ band matrix corresponding to the $S = J = 0, k = \pi$ block reported in Table 3. In this table the diagonal elements of the block are at the bottom while the elements above the diagonal (moving along columns), in the rows above. It is remarkable that the width of the band is just equal to the filling (this feature is true also for other fillings $N < 6$ [3]). One can check that the eigenvalues of the $SO(4)$ block in Table 3 are just the same as those obtained by diagonalizing the $400 \times 400$ matrix of the $S_z = 0$ space for example, the ground state energy at $t = 1, U = 1$ in both cases is $E = -6.60116$.

In closing this paper we shall estimate how the size of the $SO(4)$ blocks will grow with $f$. This can be done by counting the number $d_{f,S,J}$ of highest-lowest vectors of $SO(4)$ for a fixed $J, S$. We find that

$$d_{f,S,J} = \left( \frac{f}{c_{\pm}} \right) \left[ \left( \frac{f}{c_{-1}} \right) + \left( \frac{f}{c_{-2}} \right) \right] - \left( \frac{f}{c_{+1}} \right) \left[ \left( \frac{f}{c_{+2}} \right) + \left( \frac{f}{c_{-1}} \right) \right].$$

where $c_{\pm} = \pm (S \mp J)$ (the derivation of this formula will be given elsewhere [3]). One readily sees that Eq.8 reproduces the correct number of states associated to the filled tableaux reported in Table 1. One also checks that these states, taken with their multiplicity, reproduce the full Hilbert space i.e.

$$\frac{f!}{J!S!} \sum_{J=0}^{f/2} \sum_{S=0}^{J/2} S(S+1)J(J+1)d_{f,S,J} = 4^f.$$  

By assuming an equal splitting of the $S_f$ representations into the irreps of the translation group, we estimate the dimension of the blocks as $d_{f,S,f}/f$. Thus, for a chain with 10 sites the block characterizing the ground state at half filling is $560 \times 560$ while for a chain of 20 sites is $5 \times 10^7 \times 5 \times 10^7$. This shows that the $SO(4)$ block diagonalization allows to reduce of about two order of magnitude the sizes of the matrices constructed by using just the $S_z$ and the translational symmetry (this last being $\frac{1}{2} \left( \frac{f}{N_x} \right) \left( \frac{f}{N_y} \right)$). Moreover, it is likely that (at least in the 1D case) the band structure observed at $f = 6$ exists also at higher values of $f$. The possibility that the $SO(4)$ diagonalization leads to band matrices for arbitrary values of $f$ and $N$ is presently under investigation.

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Table Captions

Table 1
Decomposition of the filled Young tableaux corresponding to highest-lowest weight vectors of $SO(4)$ for $f = 4$ and $N = 0, 2, 4$. The splitting in terms of the irreps A, B, E, of the group $C_4$ are shown.

Table 2a
$SO(4)$ decomposition of the Hamiltonian matrix corresponding to the highest weight vectors of the $N = 2$ states in Table 1.

Table 2b
$SO(4)$ decomposition of the Hamiltonian matrix corresponding to the highest weight vectors of the $N = 4$ states in Table 1.

Table 3
Band structure of the $SO(4)$ block ($J = S = 0, k = \pi$) characterizing the ground state of the Hubbard chain with six sites. The diagonal elements of the block are reported in the row at the bottom while the elements above the diagonal (moving along columns) in the rows above.
References

[1] P W Anderson, *Science*, 235 (1987) 1196;

[2] J A White, *Phys. Rev B*, 46 (1992) 13905;

[3] A C Scott, J C Eilbeck, H Gilhøj and, *Physica D*, 78 (1994) 194;

[4] C N Yang, S C Zhang, *Mod. Phys. Lett.*, B4 (1990) 759;

[5] M Salerno, *The Hubbard model on a complete graph: exact analytical results* Z.Phys. B (1996)(to appear).

[6] M Salerno, *Exact Analytical solution for the Hubbard model with unconstrained hopping* [B Physica Scripta (1996)(to appear).

[7] see for example J F Cornwell *Group theory in Physics*. Academic Press, 1984.

[8] E H Lieb,D C Mattis, *Phys.Rev. 125, (1962) 164.

[9] M.Salerno, in preparation.
|       | $N = 0$  | $N = 2$  | $N = 4$  |
|-------|-----------|-----------|-----------|
|       | $J = 2$   | $J = 1$   | $J = 0$   |
| $S = 2$ |           |           |           |
| $S = 1$ |           |           |           |
| $S = 0$ |           |           |           |

Table 1
Table 2a

|   | $S = 0$ | $N = 2, J = 1$ | $N = 4, J = 0$ |
|---|---------|----------------|----------------|
| A | \[
\begin{pmatrix}
-\frac{8}{3}t & \frac{2}{3} \sqrt{2t} & \frac{4}{3} \sqrt{3t} \\
* & \frac{8}{3}t & \sqrt{\frac{8}{3}t} \\
* & * & U
\end{pmatrix}
\] | \[
\begin{pmatrix}
U & 2\sqrt{3}t & 2t \\
* & 2U & 0 \\
* & * & 0
\end{pmatrix}
\] | 
| B | \[
E = 0 \\
E = 0
\] | \[
\begin{pmatrix}
2U & 0 & -2t \\
* & 0 & -2\sqrt{3}t \\
* & * & U
\end{pmatrix}
\] | 
| E | $E_\pm = \frac{U}{2} \pm \sqrt{4t^2 + \left(\frac{U}{2t}\right)^2}$ | $E = U - 2t$ | $E = U + 2t$ |
### Table 2b

| \( S=1 \) | \( N=2, J=1 \) | \( N=4, J=0 \) |
|---|---|---|
| **A** | \( E = 0 \) | \( \begin{pmatrix} 0 & \sqrt{\frac{2}{3}t} & 4\sqrt{3}t \\ * & U - \frac{2}{3} & -\frac{2}{3}\sqrt{2}t \\ * & * & U + \frac{8}{3}t \end{pmatrix} \) |
| **B** | \( E = 0 \) | \( E = U \) |
| **E** | \( E_\pm = \pm 2t \) | \( E_\pm = \frac{U}{2} \pm \sqrt{4t^2 + \left(\frac{U}{2}\right)^2} \) |
| 0   | 0   | $3\sqrt{2}t$ | $3t$   | $\frac{1}{\sqrt{3}}t$ | $\frac{3}{\sqrt{2}}t$ | 0   | $\sqrt{10}t$ | 0   |
|-----|-----|-------------|--------|----------------------|-----------------------|-----|-----------|-----|
| 0   | 0   | 0           | $3t$   | $\frac{1}{\sqrt{3}}t$ | $\frac{3}{\sqrt{2}}t$ | 0   | $\sqrt{10}t$ | 0   |
| 0   | $\sqrt{3}t$ | 0           | 0      | $\sqrt{2}t$ | $\frac{1}{\sqrt{3}}t$ | 0   | $\sqrt{10}t$ | 0   |
| $4t$| 0   | 0           | $2\sqrt{2}t$ | 0       | $t$                   | 0   | $\frac{1}{\sqrt{3}}t$ | 0   |
| 0   | $t$ | $2t$        | 0      | 0                  | $\sqrt{3}t$ | $2\sqrt{2}t$ | $-t$ | 0   | 0         | 0   |
| 0   | 0   | $U$         | $U$    | $U$                 | $2U$               | $2U$ | $2U$       | $2U$ | $3U$     | $3U$ |