Proc. 13th International School on Theoretical Physics: Symmetry and Structural Properties of Condensed Matter

The Example of Using the Schur–Weyl Duality in One-Dimensional Hubbard Model

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The one-dimensional Hubbard model is discussed assuming periodic boundary conditions and the half-filling case. The Schur–Weyl duality is applied to the chain consisting of six nodes with dual actions of the unitary and symmetric groups taken separately in the spin and pseudo-spin space.

DOI: 10.12693/APhysPolA.135.1252

PACS/topics: 75.10.Pq, 03.65.Aa, 03.65.Fd

1. Introduction

The Hubbard model is one of the most fundamental one-dimensional model of interacting particles in a lattice introduced to tackle the behaviour of correlated electrons in solid. John Hubbard [1] (1931–1980) found the model to be the simplest that produces both a metallic and an insulating states of approximate behaviour of interacting electrons in a solid, depending on the value of on-site repulsion u. One of the most successful descriptions of electrons in solids is though band theory. It is based on reducing many-body interactions to an effective one-body description. The Hubbard model became especially important as it showed that for half-filling the Mott transition is reproduced, that could not be understood in terms of conventional band theory. The Hubbard model is an extension of the so-called tight-binding model, where electrons can hop between lattice sites as independent particles.

The aim of the calculations is to determine the eigenbasis adopted to the spin and the pseudo-spin symmetries for the case of the one-dimensional Hubbard model with N atoms using the Schur–Weyl duality (SWD) [2]. SWD was introduced by Schur [3] and then further developed by Weyl [4], who showed that the Young symmetrizators of symmetric groups can be used to obtain irreducible representations of a unitary group. This approach leads for the half-filling case to significance reduction of the eigenproblem of the one-dimensional Hubbard Hamiltonian.

2. The model

The dynamics of the finite set of interacting electrons, occupying the one-dimensional chain, consisted of N atoms, can be described by the Hubbard Hamiltonian in the following form

$$H = t\sum_{i\in\tilde{2}}\sum_{j\in\tilde{N}}(c^{\dagger}_{ji}c_{j+1i} + c^{\dagger}_{j+1i}c_{ji}) + u\sum_{j\in\tilde{N}} n_{j+}n_{j-}, \tag{1}$$

where $\tilde{N} = \{j = 1, 2, \ldots, N\}$ denotes the set of atoms of the chain, $\tilde{2} = \{i = +, -\}$, $n_{ji} = c^{\dagger}_{ji}c_{ji}$, and finally $c^{\dagger}_{ji}$, c_{ji} are the canonical Fermi operators, that is creation and anihilation operators of electron of spin i, on the site j. The electron hopping in the Hubbard Hamiltonian can only take place between nearest-neighbour sites, and all hopping processes have the same kinetic energy.

The set of all linearly independent vectors called *electron configurations* [5, 6] provides the initial, orthonormal basis of the Hilbert space $\mathcal{H}$. These configurations are defined by the following mapping

$$f : \tilde{N} \longrightarrow \tilde{4}, \tag{2}$$

and constitute the N-sequences of the elements from the set $\tilde{4} = \{\pm, \emptyset, +, -\}$ as follows

$$|f\rangle = |f(1)f(2)\ldots f(N)\rangle = |i_1 i_2 \ldots i_N\rangle,$$
$$i_j \in \tilde{4}, \quad j \in \tilde{N}, \tag{3}$$

where $\emptyset$ denotes the empty node, $+$ and $-$ stand for one-node spin projection equal to $\frac{1}{2}$ and $-\frac{1}{2}$, respectively, $\pm$ denotes the double occupation of the one node by two electrons with different spin projections, with

$$\tilde{4}^{\tilde{N}} = \{f : \tilde{N} \longrightarrow \tilde{4}\}, \quad \mathcal{H} = \mathrm{lc}_{\mathbb{C}}\tilde{4}^{\tilde{N}}. \tag{4}$$

3. Symmetries of the model

Since the periodic boundary condition are assumed [7], the Hamiltonian (1) has the obvious translational symmetry ($c_{N+1i} = c_{1i}$). This means that one-particle Hamiltonian of the form (1) is completely diagonalised by a Fourier transformation in the form

$$c^{\dagger}_k = \frac{1}{\sqrt{N}}\sum_{j\in\tilde{N}}\exp(\mathrm{i}2\pi kj/N)c^{\dagger}_j, \tag{5}$$

where

$$k = 0, \pm1, \ldots, \begin{cases} \pm(N/2-1), N/2, & \text{for } N \text{ even} \\ \pm(N-1)/2, & \text{for } N \text{ odd} \end{cases} \tag{6}$$

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labels the irreducible representations [5, 8] (irreps) $\Gamma_k(j) = \sum_{j \in \tilde{N}} \exp(\mathrm{i}2\pi kj/N), j \in \tilde{N}$ of the translational symmetry group C_N.

Apart from the cyclic symmetry, system reveals many other, among them, for the half-filling of the electrons, two independent SU(2) symmetries [7, 9], that is SU(2) × SU(2) in the spin and pseudo-spin space. This symmetry involves spin and charge degrees of freedom, and is related with four elementary excitation, that is spinon $\frac{1}{2}$, spinon $-\frac{1}{2}$, with respect to the spin, and holon, antiholon, with respect to the charge. The set $\tilde{4} = \{\pm, \emptyset, +, -\}$ can be decomposed into two subsets, where first $\tilde{2'} = \{\pm, \emptyset\}$ is related with the left factor of the direct product SU(2) × SU(2) of the unitary groups, and the second set $\tilde{2} = \{+, -\}$ is related with the right factor, reflecting the invariance of H under the spin rotation. Thus, one has two sets of generators, $\{S_z, S^+, S^-\}$ and $\{J_z, J^+, J^-\}$, for spin and charge, respectively.

4. The Schur–Weyl duality for one-dimensional Hubbard model in the case of half-filling

The action

$$A : \Sigma_N \times \tilde{4}^{\tilde{N}} \longrightarrow \tilde{4}^{\tilde{N}} \tag{7}$$

of the symmetric group Σ_N [5] on the set $\tilde{4}^{\tilde{N}}$ provides the orbits $\mathcal{O}_\mu$ of the group Σ_N labeled by the *weight* μ, given as the sequence of non-negative integers $\mu = (\mu_1, \mu_2, \mu_3, \mu_4)$, where the consecutive μ_i denote the number of $\pm$, $\emptyset$, $+$ and $-$ in the electron configuration, respectively, where $\sum_{i \in \tilde{4}} \mu_i = N$ and $\mu_i = |\{i_j = i | j \in \tilde{N}\}|$, $i \in \tilde{4}$. Such an orbit is invariant under the action of the symmetric group Σ_N and forms the carrier space of the transitive representation $R^{\Sigma_N : \Sigma^\mu}$, with the stabilizer Σ^μ being the Young subgroup $\Sigma^\mu = \Sigma_{\mu_1} \times \Sigma_{\mu_2} \times \Sigma_{\mu_3} \times \Sigma_{\mu_4}$, where × denotes the Cartesian product.

Since there are two independent SU(2) symmetries one can consider the action of the symmetric group Σ_N — in context of the Schur–Weyl duality [2, 10] — separately in the spin and pseudo-spin space in order to obtain the total spin S and the total pseudo-spin J. This observation holds for the system of any number N of atoms and provides two symmetric group $\Sigma_{N'}$ and $\Sigma_{N''}$ in the spin and pseudo-spin space, respectively. The actions

$$A : \Sigma_N \times \tilde{4}^{\tilde{N}} \longrightarrow \tilde{4}^{\tilde{N}}, \quad B : \mathrm{U}(4) \times \tilde{4}^{\tilde{N}} \longrightarrow \tilde{4}^{\tilde{N}} \tag{8}$$

are replaced by

$$A' : \Sigma'_N \times \tilde{2}^{\tilde{N}'} \longrightarrow \tilde{2}^{\tilde{N}'}, \quad B' : \mathrm{SU}(2) \times \tilde{2}^{\tilde{N}'} \longrightarrow \tilde{2}^{\tilde{N}'}, \tag{9}$$

in the spin space $\mathcal{H}_s = \mathrm{lc}_{\mathbb{C}} \tilde{2}^{\tilde{N}'} = h_s^{\otimes N'}$, where $h_s \cong \mathbb{C}_2$ denotes the one-node spin space, and

$$A'' : \Sigma''_N \times \tilde{2}^{\tilde{N}''} \longrightarrow \tilde{2}^{\tilde{N}''}, \quad B'' : \mathrm{SU}(2) \times \tilde{2}^{\tilde{N}''} \longrightarrow \tilde{2}^{\tilde{N}''}, \tag{10}$$

in the pseudo-spin space $\mathcal{H}_p = lc_{\mathbb{C}} \tilde{2}^{\tilde{N}''} = h_p^{\otimes N''}$, where $h_p \cong \mathbb{C}_2$ denotes the one-node pseudo-spin space. The spin and pseudo-spin spaces are isomorphic with Hilbert space of the one-dimensional Heisenberg model for the case of N' and N'' nodes of the spin chain, respectively.

Let us define some initial Hilbert space as follows

$$\mathcal{H}_{int} = \bigoplus_{(\tilde{N}', \tilde{N}'')} (\mathcal{H}_s \otimes \mathcal{H}_p),$$
$$\tilde{N}' \cup \tilde{N}'' = \tilde{N}, \tilde{N}' \cap \tilde{N}'' = \emptyset, \tag{11}$$

where N' and N'' denotes the cardinalities of the sets $\tilde{N}'$ and $\tilde{N}''$, respectively, and $(\tilde{N}', \tilde{N}'')$ stands for the pair of these two sets–each taken in ascending order. The last equations means that from now on we will label the Hilbert space (4) by $\mathcal{H}_{int}$. The space (11) can be decomposed with respect to the number of electrons in the system

$$\mathcal{H}_{int} = \bigoplus_{N_e=0}^{2N} \mathcal{H}^{N_e}, \tag{12}$$

and further with respect to the number of electron with fixed spin projection

$$\mathcal{H}^{N_e} = \bigoplus_{(N_+, N_-) = (0,0)} \mathcal{H}^{N_e}_{(N_+, N_-)}, \quad N_+ + N_- = N_e, \tag{13}$$

where N_+ and N_- denote the number of electrons with spin projection equal to 1/2 and −1/2, respectively. Since the symmetry SU(2) × SU(2) holds only for half-filling case the proper Hilbert space $\mathcal{H}$ for the case considered in the present paper is the subspace $\mathcal{H}^{N_e = N} \equiv \mathcal{H}$ of the initial space (11).

The actions (9) and (10) provide two transitive representations $R^{\Sigma_{N'} : (\Sigma_{\mu_3} \times \Sigma_{\mu_4})}$ and $R^{\Sigma_{N''} : (\Sigma_{\mu_1} \times \Sigma_{\mu_2})}$ in the spin and pseudo-spin space, respectively, where $\Sigma^{\mu'} = \Sigma_{\mu_3} \times \Sigma_{\mu_4}$ and $\Sigma^{\mu''} = \Sigma_{\mu_1} \times \Sigma_{\mu_2}$. Each transitive representation decomposes as

$$R^{\Sigma_{N'} : \Sigma^{\mu'}} \cong \sum_{\lambda' \geq \mu'} K_{\lambda' \mu'} \Delta^{\lambda'} = \sum_{\lambda' \geq \mu'} \Delta^{\lambda'}, \tag{14}$$

into irreps of the symmetric group $\Sigma_{N'}$, with the partition $\lambda' \vdash N'$ defining the shape of the corresponding irrep $\Delta^{\lambda'}$, where $K_{\lambda' \mu'}$ are the famous Kostka numbers, equal to 1 in case of two-dimensional one-node space, the sum runs over all partitions λ' of N' which are not smaller than μ' in the dominance order, and N' denotes the number of appropriate one-node spin spaces h_s. For the pseudo-spin space with N'' number of appropriate one-node pseudo-spin spaces h_p by analogy to (14) the following decomposition holds

$$R^{\Sigma_{N''} : \Sigma^{\mu''}} \cong \sum_{\lambda'' \geq \mu''} K_{\lambda'' \mu''} \Delta^{\lambda''} = \sum_{\lambda'' \geq \mu''} \Delta^{\lambda''}, \tag{15}$$

into irreps of the symmetric group $\Sigma_{N''}$, with the partition $\lambda'' \vdash N''$ defining the shape of the corresponding irrep $\Delta^{\lambda''}$.

5.The example of the chain consisted of six nodes

In the present paper we examine the example of the chain with six nodes $N = 6$ at the half-filling, thus the weights are as follows

$$\begin{array}{ccccc} N' & N'' & N_+ & N_- & \mu \\ \hline 6 & 0 & 6 & 0 & (0,0,6,0) \\ & & 5 & 1 & (0,0,5,1) \\ & & 4 & 2 & (0,0,4,2) \\ & & 3 & 3 & (0,0,3,3) \\ & & 2 & 4 & (0,0,2,4) \\ & & 1 & 5 & (0,0,1,5) \\ & & 0 & 6 & (0,0,0,6) \\ \hline 4 & 2 & 5 & 1 & (1,1,4,0) \\ & & 4 & 2 & (1,1,3,1) \\ & & 3 & 3 & (1,1,2,2) \\ & & 2 & 4 & (1,1,1,3) \\ & & 1 & 5 & (1,1,0,4) \\ \hline 2 & 4 & 4 & 2 & (2,2,2,0) \\ & & 3 & 3 & (2,2,1,1) \\ & & 2 & 4 & (2,2,0,2) \\ \hline 0 & 6 & 3 & 3 & (3,3,0,0) \end{array} \tag{16}$$

The dimension of the initial Hilbert space $\mathcal{H}_{int}$ given by the Eq. (11) for the case of the chain consisted of six nodes $N = 6$ is equal to $4096 = 4^6$. The dimension of the proper Hilbert space given as the subspace $\mathcal{H}^{N_e=N=6}$ of the initial Hilbert space can be calculated as follows

$$\mathcal{H} = \mathcal{H}^{N_e=6} = \bigoplus_{(N_+,N_-)=(0,0)} \mathcal{H}^{N_e=6}_{(N_+,N_-)},$$

$$N_+ + N_- = 6. \tag{17}$$

Thus the dimension of the Hilbert space $\mathcal{H}$ is equal to

$$\dim\mathcal{H} = \dim\mathcal{H}^6_{(6,0)} + \dim\mathcal{H}^6_{(5,1)} + \dim\mathcal{H}^6_{(4,2)}$$
$$+\dim\mathrm{H}^6_{(3,3)} + \dim\mathcal{H}^6_{(2,4)} + \dim\mathcal{H}^6_{(1,5)} + \dim\mathcal{H}^6_{(0,6)}$$
$$\dim\mathcal{H} = 1 + 36 + 225 + 400 + 225 + 36 + 1 = 924. \tag{18}$$

The result above can be written as follows

$$2^6 + \binom{2}{1}(2^4)\binom{6}{4} + \binom{4}{2}(2^2)\binom{6}{2} + \binom{6}{3},$$

since the multiplicity of deploying of N' spin atoms and N'' pseudo-spin atoms on the chain consisted of $N = N' + N''$ atoms is equal to

$$\tau = \binom{N}{N'} = \binom{N}{N''}.$$

The decomposition of the transitive representations of the actions (9) and (10) of the symmetric group Σ_6 into irreducible representations provides the irreducible basis with specified values of total spin S and the total pseudo-spin J. For example, the total number of states for the case of $S_z = 1$ and $J_z = 0$ (the ninth row of the summary (16)) can be calculated as follows

$$\dim\left[(R^{\{1^2\}} \otimes R^{\{3\,1\}})\right] \times \tau = \tag{19}$$
$$\dim\left[(\Delta^{\{2\}} \oplus \Delta^{\{1^2\}}) \otimes (\Delta^{\{4\}} \oplus \Delta^{\{3\,1\}})\right] \times \tau = 8 \times \tau$$

where the first and the second transitive representations correspond to the pseudo-spin and the spin space, respectively, since $N'' = 2$ and $N' = 4$. The multiplicity of deploying of N' spin atoms and N'' pseudo-spin atoms on the chain consisted of $N = N' + N''$ atoms is equal to $\tau = 15$, thus the number of states for the considered case is equal to 120 and together with the number of states for $N' = 6$ ($N'' = 0$) and $N' = 2$ ($N'' = 4$) for the same S_z and J_z contributes to the number 225 of the Eq. (18).

6. Conclusions

We presented the application of the Schur–Weyl duality in the one-dimensional Hubbard model in the case of half-filling for the example of six atoms. We introduced the spin and pseudo-spin space in order to obtain the total spin S and the total pseudo-spin J. We used the concept of initial Hilbert space which provides the proper Hilbert space of the considered system as its subspace. The calculations are significant since the obtained results lead to a significant reduction in the size of the Hubbard Hamiltonian.

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