$T \geq 0$ properties of the infinitely repulsive Hubbard model for arbitrary number of holes.

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Abstract

Based on representations of the symmetric group $S_N$, explicit and exact Schrödinger equation is derived for $U = \infty$ Hubbard model in any dimensions with arbitrary number of holes, which clearly shows that during the movement of holes the spin background of electrons plays an important role. Starting from it, at $T = 0$ we have analyzed the behaviour of the system depending on the dimensionality and number of holes. Based on the presented formalism thermodynamic quantities have also been expressed using a loop summation technique in which the partition function is given in terms of characters of $S_N$. In case of the studied finite systems, the loop summation have been taken into account exactly up to the 14th order in reciprocal temperature and the results were corrected in higher order based on Monte Carlo simulations. The obtained results suggest that the presented formalism increase the efficiency of the Monte Carlo simulations as well, because the spin part contribution of the background is automatically taken into account by the characters of $S_N$. 

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I. INTRODUCTION

The physics of holes moving in a background build up from a great number of electrons has received much attention in the last decade given by the connection of this problem with main questions arising from the study of strongly correlated systems (Chernyshev and Leung 1999). Developments in several fields underline this aspect: behaviour in antiferromagnetic background (Anderson 1997), metal-insulator transition (Trugman 1990 a), doping effects (Loius et al. 1999), ferromagnetism (Kollar et al. 1996), high $T_c$ superconductivity (Trugman 1998), colossal magnetoresistance (Ishihara et al. 1997), spiral states (Watanabe and Miyashita 1999), generalized-statistics (Long and Zotos 1992), pairing mechanism and bound-states (Trugman 1990 b), polaronic effects (Louis et al. 1993), are main examples to be mentioned. From the theoretical side the Hubbard type models are especially involved in the theoretical description starting from infinite on-site repulsion (Nagaoka 1966), finite Hubbard interaction (Süttö 1991), and continuing with the inclusion of spin-independent interactions (Tasaki 1989), extensively extended versions (Kollar et al. 1996), degenerated orbitals (Shen and Wang 1999) and limiting cases like the $t – J$ model in one-band (Chernyshev and Leung 1999), or multi-band versions (Shen and Wang 1999). The theoretical descriptions started with the 1-hole problem discussed by Nagaoka (Nagaoka 1966), which has been continued with two-holes studies (Kuz’min 1993), and many-hole analyses in various configurations and circumstances (Mattis 1986, Doucot and Wen 1989, Barbieri et.al. 1990, Tóth 1991, Tian 1991). Despite the huge intellectual effort spent in the field exact results related to the mentioned problem are extremely rare (Mattis 1986) and concern only the 1-hole Nagaoka-state (Nagaoka 1966) and its possible extensions (Tasaki 1989, Süttö 1991, Tóth 1991). However, in the above enumerated concrete applications mostly multi-hole descriptions are needed mainly in strong-coupling limit. These situations have been treated in the literature based on various approximations (acceptable in restricted conditions) like complete separation of charge and spin degrees of freedom (Kuz’min 1993), extended Gutzwiller wave-functions (Gebhard and Zotos 1991), canonical transformations
(Chernyshev et al. cond-mat 9806018), generalization of 1D results to higher dimensions (Doucot and Wen 1989), restrictions related to the number of holes (Barbieri et al. 1990), unrestricted Hartree-Fock (Loius et al. 1999), etc., or numerical procedures like exact diagonalization on small clusters (Takahashi 1982), and diagonalization within a retained portion of the Hilbert space (Trugman 1998). We witnessed also studies on specific problems like ferromagnetism (Vollhardt et al. 1998).

On the background of the mentioned large spectrum of description attempts, in this paper we are presenting an unifying aspect of the hole-motion in the simple one-band Hubbard model in the limit of infinitely large on-site repulsion $U$. For this reason first of all we have deduced and presented an exact and explicit Schrödinger equation for an arbitrary number of holes in the analyzed model. This equation clearly underlines the role played by the charge and spin degrees of freedom during the movement of the holes in the $U = \infty$ Hubbard model, being mathematically based on the representations of the symmetric group $S_N$ of degree $N$, where $N$ represents the number of electrons within the system. Advantages of the presented description are underlined by the observations that: a) the emerging matrix elements can be find (or deduced in case of larger systems) from standard textbooks of the group theory, and b) the analysis reduced the concrete equation to be solved in subspaces fixed by a given, but arbitrary total system spin $S$ of the initial large Hilbert space, allowing comfortable numerical applications.

After this step, and concrete applications of the deduced equation related to the $T = 0$ spectrum and physical properties of small samples, we turn on the study of $T \neq 0$ properties by showing how the presented formalism helps the deduction of the partition function $Z$ based on the characters of the representations of the symmetric group (again accessible from standard text-books in group theory). The emerging coefficients in $Z$ can be reduced to coefficients easily obtainable from numerical methods, being related to the number of different loops with fixed length that can be drawn in the studied system connecting its lattice sites. The procedure is able even to increase the efficiency of the usual Monte Carlo simulation methods. Starting from the deduced formulas, we are presenting some examples
of the $T \neq 0$ behaviour of the two-hole case.

Our results clearly underline that in the infinitely repulsive Hubbard model the movement of holes is intimately influenced by the spin-background of the electrons. As a consequence, in describing this process in the general case, the charge and spin degrees of freedom cannot be entirely separated.

The remaining part of the paper is organized as follows: Sec. II. describes the studied model and introduces the used notations, Sec. III. presents the basis of the Hilbert space used during the paper, Sec. IV. describes the action of the Hamiltonian on the basis vectors, Sec. V. presents the deduced Schrödinger equation together with applications, Sec. VI. concentrates on $T \neq 0$ properties and emphasises the advantages of the presented formalism in deducing thermodynamic quantities like partition function, thermodynamic potential, specific heat, expectation value of the total spin, Sec. VII. presents a summary of the paper, and an Appendix containing the mathematical details closes the presentation.

II. THE MODEL AND NOTATIONS USED

Our starting Hamiltonian ($\hat{H}$) describes the one-band Hubbard model in $U = \infty$ limit. Given by the absence of doubly occupied sites in the lattice, $\hat{H}$ becomes

$$\hat{H}_\infty = \sum_{i,j} t_{ij} \hat{H}^i_j = \sum_{i,j} t_{ij} \hat{P} \left( \sum_{\sigma} \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} \right) \hat{P},$$

(1)

where $t_{ij} = -t$ are hopping matrix elements for nearest neighbour sites (otherwise $t_{ij} = 0$). The operators $\hat{c}^\dagger_{i,\sigma}$ ($\hat{c}_{i,\sigma}$) creates (annihilates) an electron with spin $\sigma$ at lattice site $i$, and $\hat{n}_i = \sum_{\sigma} \hat{n}_{i,\sigma}$ represents particle number operator. The double occupancy is projected out by $\hat{P} = \sum_i (1 - \hat{n}_i \hat{n}_i)$. For convenience, we denote the lattice by $\Lambda$, the number of the lattice sites by $N_\Lambda$, the number of electrons by $N$, so the number of holes becomes $N_h = N_\Lambda - N$. Being also interested in magnetic properties, we present below the notations and definitions related to spin characteristics. The total spin operator is taken as

$$\hat{S} = \frac{1}{2} \sum_{i \in \Lambda} \sum_{\sigma,\sigma'} \hat{c}^\dagger_{i,\sigma} \tau_{\sigma,\sigma'} \hat{c}_{i,\sigma'}$$

(2)
where $\tau = (\tau^x, \tau^y, \tau^z)$ are the Pauli matrices. Furthermore we have $\hat{S}^\pm = \hat{S}^x \pm i \hat{S}^y$ and $\hat{S}^2 = (\hat{S}^x)^2 + (\hat{S}^y)^2 + (\hat{S}^z)^2$. We denote by $S^z$ the eigenvalue of $\hat{S}^z$ and by $S(S + 1)$ the eigenvalue of $\hat{S}^2$. The quantity $S$ represents the total spin of the state described.

**III. THE HILBERT SPACE VECTOR-BASIS USED**

Now we prepare a basis for a sector of the Hilbert space of the system with a fixed $N_h$ number of holes and a given $S^z$ projection of the total spin. We start from Hilbert space vectors characterized by the position of holes $h_1, \ldots, h_{N_h}$, and the spin configuration of the electrons situated in single occupied states $\{\sigma_i\}_{i \in \Lambda \setminus \{h_1, \ldots, h_{N_h}\}}$, defined as

$$|\psi_{\{h\},\{\sigma\}}\rangle = \prod_{i \in \Lambda \setminus \{h_1, \ldots, h_{N_h}\}} \hat{c}_{i,\sigma_i}^\dagger |0\rangle,$$

where the product is taken over all the occupied sites in $\Lambda$, and $|0\rangle$ represents the bare vacuum with no fermions present. For mathematical convenience, we introduce the convention that the elements of $\Lambda$ are building up an ordered set (i.e. the lattice sites are numbered) and the product in Eq.(3) follows this order. As a consequence, the product of creation operators from Eq.(3) is written in increasing order with respect to lattice indices. Let us introduce now the function $\mathcal{R} : \{1, \ldots, N_\Lambda\} \to \{1, \ldots, N_\Lambda\}$ that performs a regroupation of lattice site positions, maintaining however their initial numbering. By definition, $\mathcal{R}$ gives the indices of occupied lattice sites in increasing order for the first $N$ numbers in the $\{1, \ldots, N_\Lambda\}$ set, and introduces the indices of the empty sites in arbitrary order for the last $N_h$ positions of the mentioned set (we underline, $N_\Lambda = N + N_h$). The numbering of hole positions obtained after the action of $\mathcal{R}$ being arbitrary, $\mathcal{R}$ itself is not uniquely defined. Using it, $|\psi_{\{h\},\{\sigma\}}\rangle$ becomes

$$|\psi_{\{h\},\{\sigma\}}\rangle = \prod_{i=1}^{N} \hat{c}_{\mathcal{R}(i),\sigma_{\mathcal{R}(i)}}^\dagger |0\rangle.$$

In order to describe the spin configuration with a fixed $S^z$ projection of the total spin, we observe that $S^z$ can be characterized by permutations $\mathcal{P} \in S_N$ of the symmetric group of
degree $N$. Indeed, the set $\{ \sigma_i \}_{i \in \Lambda \setminus \{ h_1, \ldots, h_{N_h} \}}$ represents in fact a permutation of $N_\uparrow$ symbols $\uparrow$ and $N_\downarrow = N_\uparrow - 2S^z$ symbols $\downarrow$ (see Appendix). Using $\mathcal{P}$, the spin configuration can be denoted as $(\sigma_i)_{i \in \Lambda \setminus \{ h_1, \ldots, h_{N_h} \}} = (\sigma(\mathcal{P}(i)))_{i = 1}^N$, where the function $\sigma$ defined by $\sigma(i) := \uparrow$ if $i = 1, \ldots, N_\uparrow$ and $\sigma(i) := \downarrow$ if $i = N_\uparrow + 1, \ldots, N$. With the introduced notations the basis vectors of the Hilbert space with fixed number of holes $N_h$ and fixed total spin projection $S^z$ can be written as

$$| \mathcal{R}, \mathcal{P} \rangle = \prod_{i=1}^N \hat{c}_{\mathcal{R}(i), \sigma(\mathcal{P}(i))}^\dagger |0\rangle.$$  (5)

The subspaces generated by vectors $\{ | \mathcal{R}, \mathcal{P} \rangle \}_{\mathcal{P} \in S_N}$ with different $\mathcal{R}$ are different but isomorphic parts of the whole Hilbert space of the system. Let us denote by $\mathcal{H}_s^{S^z}$ the Hilbert space which is isomorphic with all subspaces generated by $\{ | \mathcal{R}, \mathcal{P} \rangle \}_{\mathcal{P} \in S_N}$ with arbitrary but fixed $\mathcal{R}$ and $S^z$ (see Appendix). Similarly $\mathcal{H}_c$ denotes the Hilbert space which is isomorphic with all spaces generated by vectors $| \mathcal{R}, \mathcal{P} \rangle$ with arbitrary but fixed $\mathcal{P}$ and $S^z$. We mention that independently on $S^z$, $\mathcal{H}_c$ represents in fact a Hilbert space of a system of hard core spinless particles. With this notation the whole Hilbert space of the system $\mathcal{H}$ is a direct sum over $S^z$ sectors $\mathcal{H} = \oplus_{S^z} (\mathcal{H}_c \otimes \mathcal{H}_s^{S^z})$. We underline, that introducing the notation $\mathcal{H}_s = \oplus_{S^z} \mathcal{H}_s^{S^z}$, we have only $\mathcal{H} \cong \mathcal{H}_c \otimes \mathcal{H}_s$.

In the remaining part of the paper we denote an arbitrary element of $\mathcal{H}_s^{S^z}$, $\mathcal{H}_s$ and $\mathcal{H}_c$ by $\varphi_s^{S^z}$, $\varphi_s$ and $\varphi_c$, respectively. Furthermore the basis vectors of $\mathcal{H}_c$ will be written as $| \mathcal{R} \rangle$, and the basis vectors of $\mathcal{H}_s^{S^z}$ as $| \mathcal{P} \rangle$. With these notations the basis vectors that we have are $| \mathcal{R}, \mathcal{P} \rangle = | \mathcal{R} \rangle \otimes | \mathcal{P} \rangle$. The states $| \mathcal{R} \rangle$ describe in fact the charge distribution and $| \mathcal{P} \rangle$ the spin configuration. We have to mention that Eq.(3) has to be used with care because it contains redundant information. Every $\mathcal{R} \in S_{N_\Lambda}$ and $\mathcal{P} \in S_N$ uniquely define a basis vector $| \mathcal{R} \rangle \otimes | \mathcal{P} \rangle$, but several different pairs of permutations define the same basis vector. Because of this reason indexing these basis vectors by integers, in the case of the basis set $\{ | \mathcal{R}_i \rangle \} \subset \mathcal{H}_c$ the index $i$ goes up to $\binom{N_\Lambda}{N}$ and not to $N!$. Similarly, the basis set $\{ | \mathcal{P}_i \rangle \} \subset \mathcal{H}_s^{S^z}$ has $\binom{N}{N/2+S^z}$ different elements. The reason why we express the basis vectors in term of permutations is detailed in the Appendix: the Hilbert space of the
spin configurations for fixed $N$ and $S^z$ is isomorphic with a proper right ideal of the group algebra $C[S_N]$ of the symmetric group $S_N$.

We emphasize that the Hamiltonian presented in Eq.(1) cannot be written in the product form $\hat{H}_\infty \neq \hat{H}_c \otimes \hat{H}_s$ and the effect of the Hamiltonian on $H_s^{S^z}$ depends on the hole configuration (charge distribution) $| P \rangle$. However, contrary to $\hat{c}$ Eq.(1), only the term $\hat{c}$ by a fixed total spin $S$, i.e. on $| R \rangle \otimes | P \rangle$. In fact we have $\hat{H}_{ij}^{ij} = \hat{H}_{c}^{ij} \otimes \hat{H}_{s}^{ij}$ ( $R$ ), therefore the eigenstates of $\hat{H}$ in general case cannot be written in the form $| \varphi_c \rangle \otimes | \varphi_s \rangle$. As a consequence, there is no a priori charge spin separation taken into account at the level of the description. However, contrary to $\hat{H}$, the effect of spin operators does not depend on $| R \rangle$, i.e. on $H_c$. This is why the decomposition of the Hilbert space into sectors characterized by a fixed total spin $S$ can be done within $H_s = \oplus_{S^z} (\oplus_{S=S} H_s^{S^z})$. Denoting by $\varphi^{S^z,S}$ an element of $H^{S^z,S} = H_c \otimes H_s^{S^z}$, an arbitrary common eigenvector of $\hat{S}^z$ and $\hat{S}^2$ in the sector of fixed number of holes can be written as $\varphi_c \otimes \varphi^{S^z,S}$.

IV. ACTING WITH THE HAMILTONIAN ON BASIS VECTORS.

The contribution $\hat{H}_\infty^{ij}$ of the Hamiltonian from Eq.(1) has non-vanishing effect on a basis vector from Eq.(3) only if $i$ represents a hole position and $j$ an electron position, i.e. $1 \leq R^{-1}(i) \leq N$ and $N + 1 \leq R^{-1}(j) \leq N_A$. Furthermore, regarding the spin sum in Eq.(1), only the term $\hat{c}_{i,\sigma'}^{\dagger} \hat{c}_{j,\sigma'}$ of $\hat{H}_\infty^{ij}$ has non-vanishing effect in which $\sigma' = \sigma(\mathcal{P} R^{-1}(j))$. Using the notation $\tilde{j} = R^{-1}(j)$, we obtain

$$
\hat{H}_\infty^{ij} ( | R \rangle \otimes | \mathcal{P} \rangle ) = \hat{c}_{i,\sigma(\mathcal{P})(j)}^{\dagger} \hat{c}_{j,\sigma(\mathcal{P})(j)} \prod_{l=1}^{N} \hat{c}_{R(l),\sigma(\mathcal{P}(l))}^{\dagger} | 0 \rangle = \hat{c}_{i,\sigma(\mathcal{P})(j)}^{\dagger} \hat{c}_{j,\sigma(\mathcal{P})(j)} \prod_{l=1}^{N} \hat{c}_{R(l),\sigma(\mathcal{P}(l))}^{\dagger} | 0 \rangle
$$

$$
\cdots \hat{c}_{R(j-1),\sigma(\mathcal{P}(j-1))}^{\dagger} \hat{c}_{j,\sigma(\mathcal{P}(j))} \hat{c}_{R(j+1),\sigma(\mathcal{P}(j+1))} \cdots \hat{c}_{R(N),\sigma(\mathcal{P}(N))}^{\dagger} | 0 \rangle
$$

$$
= \hat{c}_{R(1),\sigma(\mathcal{P}(1))}^{\dagger} \cdots \hat{c}_{R(j-1),\sigma(\mathcal{P}(j-1))}^{\dagger} \hat{c}_{j,\sigma(\mathcal{P}(j))} \hat{c}_{R(j+1),\sigma(\mathcal{P}(j+1))} \cdots \hat{c}_{R(N),\sigma(\mathcal{P}(N))}^{\dagger} | 0 \rangle
$$

$$
= \prod_{l=1}^{N} \hat{c}_{R(l),\sigma(\mathcal{P}(l))}^{\dagger} | 0 \rangle
$$

(6)

where $\mathcal{P}^{(i,j)}$ represents the transposition that interchanges the indices $i$ and $j$. The result cannot be written in the form $| \mathcal{P}^{(i,j)} R \rangle \otimes | \mathcal{P} \rangle$, because the permutation $\mathcal{P}^{(i,j)} R$ does not meet the requirements regarding the site ordering presented after Eq.(3). Indeed, the
creation operators are no more situated within the product in increasing order with respect
to their lattice indices because $\hat{c}_{i,\sigma(\mathcal{P}(j))}^\dagger$ is situated in a wrong place. To overcome this
situation, let us introduce the cyclic permutation $\mathcal{C}(\mathcal{R} ; i , j ) \in S_N$ which rearranges
the $N$ pieces of operators of the last row of Eq.(6) in the required order by moving the
$\hat{c}_{i,\sigma(\mathcal{P}(j))}^\dagger$ operator positioned at site $\tilde{j}$ to the required position within the product. In the
$i < j$ ($i > j$) case, for this purpose $\mathcal{C}(\mathcal{R} ; i , j )$ interchanges the $\hat{c}_{i,\sigma(\mathcal{P}(j))}^\dagger$ operator with
previous (following) operators. The last operator with which we interchange, is situated in
the position $\mathcal{R}^{-1}(i’)$. Here, in the $i > j$ case $i’$ is the least index among the indices greater
than $i$ for which $\mathcal{R}^{-1}(i’) \leq N$, and in the $i < j$ case $i’$ is the greatest index among the
indices smaller than $i$ for which $\mathcal{R}^{-1}(i’) \leq N$. In other words $i’$ labels the occupied lattice
site whose index is closest to $i$ among the indices situated between $i$ and $j$. Now we have
\[ \mathcal{C}(\mathcal{R} ; i , j ) = \mathcal{C}^{(\mathcal{R}^{-1}(j)\rightarrow\mathcal{R}^{-1}(i’))} . \] (7)

It can be observed that we get the ordered sequence of the operators in Eq.(6) if we permute
their indices by $\mathcal{C}^{-1}(\mathcal{R} ; i , j )$. Given by this, also a sign-change $(-1)^{\mathcal{C}(\mathcal{R};i,j)}$ is obtained,
where $|\mathcal{C}|$ has the meaning of the parity of the permutation. Based on the presented
properties we obtain
\[ \hat{H}_i^{ij} \left( |\mathcal{R}\rangle \otimes |\mathcal{P}\rangle \right) = \left(-1\right)^{\mathcal{C}(\mathcal{R};i,j)} \prod_{l=1}^{N} \hat{c}_{\mathcal{P}(i,j)\mathcal{R}^{-1}(\mathcal{R};i,j)(l),\sigma(\mathcal{P}(i,j)(l))}^\dagger |0\rangle \]
\[ = |\mathcal{P}(i,j)\mathcal{R}^{-1}(\mathcal{R} ; i , j )\rangle \otimes \left(-1\right)^{\mathcal{C}(\mathcal{R};i,j)} |\mathcal{P}\mathcal{C}^{-1}(\mathcal{R} ; i , j )\rangle . \] (8)

The difference between the hole configuration described by the permutation $\mathcal{R}$ and
$\mathcal{P}(i,j)\mathcal{R}^{-1}(\mathcal{R} ; i , j )$ lies in the position of one hole, which has been moved from site
$i$ to site $j$. This shows that the holes are moved by the Hamiltonian as if they were hard
core bosons, while the spin configuration is changing depending on the actual hole config-
uration. The Hilbert space generated by the vectors $|\mathcal{R}\rangle$ is actually the Hilbert space of
$N_h$ hard core bosons ($|\mathcal{R}\rangle$ describes the state in which $N_h$ particles are situated in the
$\mathcal{R}(N+1), \ldots, \mathcal{R}(N_A)$ lattice sites positions). Therefore, we write the effect of the Hamil-
tonian as $\hat{H}_i^{ij} |\mathcal{R}\rangle$, taking into account supplementary the effect on the spin configuration.
According to the Appendix, the effect on the spin configuration can be described with a linear operator $T^{S^z}[C(\mathcal{R}; i, j)]$ where $T^{S^z}$ is a representation of $S_N$ uniquely determined by $S^z$. Based on these considerations, the effect of the Hamiltonian on the basis defined by Eq.(5) can be given as

$$\hat{H}_\infty (|\mathcal{R}\rangle \otimes |\mathcal{P}\rangle) = \sum_{i,j} t_{ij} \hat{H}_{b,\infty}^{ij} |\mathcal{R}\rangle \otimes T^{S^z}[C(\mathcal{R}; i, j)] |\mathcal{P}\rangle.$$  \(9\)

Starting from Eq.(9) we analyze below the Schrödinger equation describing the behavior of the system.

**V. THE SCHRÖDINGER EQUATION**

Due to the fact that the system is invariant under the SU(2) global rotations, in the spin space the Hamiltonian and $\hat{S}^2$ are simultaneously diagonalizable. Therefore the spin eigen-subspaces are invariant under the effect of the Hamiltonian. The effect of the Hamiltonian on $\mathcal{H}_{s}^{S^z,S}$ can be described by a $T_S$ representation of the symmetric group independently of $S^z$ (see Appendix). Let us denote by $(T_S[\mathcal{P}])_{nm}$ the matrix elements of the operator $T_S[\mathcal{P}]$ in an orthogonal and normalized basis of $\mathcal{H}_{s}^{S^z,S}$ with arbitrary $S^z$ (denoted by $\{ |b^S_n\rangle \}$), and by $(H_{b,\infty}^{ij})_{kl} = \langle \mathcal{R}_k | \hat{H}_{b,\infty}^{ij} | \mathcal{R}_l \rangle$ where $\mathcal{R}_k$, $\mathcal{R}_l \in \{ |\mathcal{R}_i\rangle \}_{i=1}^{N_{\Lambda}}$ are basis vectors indexed by integers in $\mathcal{H}_c$. Now the Schrödinger equation becomes

$$\sum_{l,m} \alpha_{lm} \sum_{i,j} t_{ij} (H_{b,\infty}^{ij})_{kl} (T_S[C(\mathcal{R}_i; i, j)])_{nm} = E \alpha_{kn}$$  \(10\)

Eq.(10) gives the energy eigenvalues $E$ connected to the eigenstates with given total spin $S$. The $\alpha_{kn}$ coefficients in Eq.(10) represent the coordinates of the energy eigenstate $E$ in the basis $|\mathcal{R}\rangle \otimes |b^S\rangle$ given as

$$|\psi_{E,S}\rangle = \sum_{kn} \alpha_{kn} |\mathcal{R}_k\rangle \otimes |b^S_n\rangle$$  \(11\)

We have to mention that essentially the same wave vectors as presented in Eq.(11) has been used by Long and Zotos (Long and Zotos 1993) in the study of the stability of the Nagaoka state, without however to write an explicit Schrödinger equation for it.
It can be seen from Eq.(11) that the matrix elements of the Hamiltonian between spin states depend also on the hole configuration $\mathcal{R}$, i.e. charge distribution, so dynamically the spin degrees of freedoms are not separated from the charge degrees of freedom. At the level of the basis states however, we have the possibility to treat them separately and this allows us to write the Schrödinger equation in the form of Eq.(10). We also can use Eq.(10) for exact numerical diagonalizations. The main advantage of Eq.(10) is that the matrix elements of the starting Hamiltonian have been reduced to a direct sum of matrices related to the invariant subspaces $\mathcal{H}_{S,S_z}^S$. Because of this reason, in concrete applications we need to solve the eigenvalue problem of Eq.(10) in a relatively small Hilbert space instead of $\mathcal{H}_{S_z}^S$ which is much larger. For concrete application the following indications are needed in order to use Eq.(10): The matrix elements of the hard core boson Hamiltonian can be easily calculated and for small number of electrons the matrix elements of the representation $T_S$ is given in mathematical textbooks (see for example Hamermesh 1962, Table 7.3). For greater $N$ values their clear calculation procedure is also available from same sources (see e.g. Hamermesh 1962, Section 7.7).

Eq.(10) shows explicitly the role played by the total spin $S$ in the Schrödinger equation. For example in the case of $S = S_{max}$, the representation $T_{S_{max}}$ is the alternating representation. In this case the dimension of $\mathcal{H}_{S_z}^{S_z,S_{max}}$ is 1, and the matrix representing every even permutation is 1 and every odd permutation is $-1$. Because of this reason hard core fermions with maximal spin do not differ from spinless fermions (see also Long and Zotos 1993). The on-site interaction has no effect on spinless fermions therefore there is no differention between hard core and free particles in this case.

Another simple example is the 1D case with open boundary conditions. Numbering the sites of the chain in order one after another, the form of every nearest neighbour pair is simply $\langle i, i+1 \rangle$ in this case, and we have $C(\mathcal{R}; i, i+1) = 1 \in S_N$ whose matrix is the unity matrix for arbitrary representation. Therefore there is no difference between hard core bosons and fermions, so the energy spectrum is independent of the spin of particles, only every energy eigenvalue is $(2S + 1)^N$ fold degenerate, $S$ being the spin of particles.
If $D > 1$ and $S^z \neq S_{\text{max}}$ than the effect of the Hamiltonian on the spin background is highly nontrivial, and influences the mobility and interaction of holes. A such type of situation was analyzed by numerical technique by Trugman (Trugman 1998). He showed that on Néel type antiferromagnetic background one hole is mobile but two holes are less mobile than it was previously considered. This is due in fact in the language presented here by the permutation possibilities of spin positions with mobile hole positions. Trugman’s results underlined as well that the effect of the Hamiltonian is clearly seen also on the spin background, which cannot be treated entirely separated from the movement of the holes within the system.

We note that the Schrödinger equation Eq.(10) essentially differs from Kuzmin’s equation (Kuz’min 1993) for the purpose to solve the two hole problem on singlet background. In the mentioned reference the Schrödinger equation has been solved supposing implicitly that the Hamiltonian has no effect on the spin degrees of freedom i.e. spin background. From Eq.(10) it can be seen that this is correct in the case of a hard core boson system only. This explains why Kuz’min obtains the result that the Nagaoka state (the fully polarized ferromagnetic state) is degenerated with the singlet state even in the one hole case, in contradiction with the Nagaoka’s original result (Nagaoka 1966). In one hole case the spectrum given by Kuz’min is really related to a hard core spinless boson system spectrum, which is equivalent with the spectrum of a spinless fermion system. This last one, on its turn, is equivalent with the $S_{\text{max}}$ spectrum of our original electron system as presented above. The first equivalence is due to the fact that for hard core spinless particles (both bosons and fermions) the $N$ hole problem is equivalent with the $N$ particle problem, and in the one particle case the statistics is unimportant. For more than one hole it is not the same whether we deal with bosons or fermions even for hard core interaction. The ground state energy of the bosons is always smaller (Long and Zotos 1993). In order to exemplify, we mention that the equality presented by Kuz’min

$$0 = \sum_k \frac{1}{E - (\epsilon_k + \epsilon_{P-k})}$$  \hspace{1cm} (12)
gives the spectrum of a spinless hard core boson system consisting of two particles (or equivalently two holes). Here $\epsilon_k$ is the one particle dispersion relation and $P$ is the total momentum of the system. For the ground state energy of the simplest non-trivial two dimensional case, the $2 \times 3$ lattice, Eq.(12) gives $E_0 = -6.6468$ while from Eq.(10) one find $E_0 = -6$ which connected to the $S = S_{\text{max}} = 2$ value of the total spin, and $E_{S=0}^{\text{min}} = -5.0212$ is the lowest energy value on singlet background. Furthermore we note that in the two particle case the spectrum of hard core spinless boson system is identical with the spin 1/2 fermion system's singlet spectrum, therefore it can be computed using Eq.(12). However, as presented here, in the $S \neq S_{\text{max}}$ case the behaviour of the system described by Eq.(1) cannot be described by hard core particles and independent spin degrees of freedom. This is the reason why the $N$ particle and the $N$ hole problems are not generally equivalent, and the behaviour of few holes is more complicated than the behaviour of few particles.

VI. THERMODYNAMIC QUANTITIES

An asset of the representation presented in Eq.(1) is that the trace of $(\hat{H}_\infty)^\dagger$ over the spin degrees of freedom can be computed with this relation exactly. This allows us to calculate expectation values at $T \neq 0$ of different thermodynamic quantities. The procedure is presented as follows.

A. The partition function and total spin

If we are interested in the magnetic properties of the model Eq.(1), we may express for example the expectation value of the square of the total spin. We have

$$\langle \hat{S}^2 \rangle = \frac{1}{Z} \sum_{S} S (S+1) \sum_{-S \leq S^z \leq S} \text{Tr} \hat{H} S^z S e^{-\frac{\hat{H}kT}{\hbar}} = \frac{1}{Z} \sum_{S} 3 (S^z)^2 \text{Tr} \hat{H} S^z S e^{-\frac{\hat{H}kT}{\hbar}},$$

(13)

where the partition function is given by
\[ Z = \sum_{S} \sum_{-S \leq S^z \leq S} \text{Tr}_{\mathcal{H}^{S^z}} e^{-\frac{\beta S^z}{kT}} = \sum_{S^z} \text{Tr}_{\mathcal{H}^{S^z}} e^{-\frac{\beta S^z}{kT}}. \] (14)

In Eqs. (13, 14) we used the fact that \( \text{Tr}_{\mathcal{H}^{S^z}} e^{-\frac{\beta H_{\infty}}{kT}} \) does not depend on \( S^z \) due to the SU(2) symmetry, therefore \( \sum_{S^z} \text{Tr}_{\mathcal{H}^{S^z}} e^{-\frac{\beta H_{\infty}}{kT}} = \text{Tr}_{\mathcal{H}^{S^z}} e^{-\frac{\beta H_{\infty}}{kT}} \) for arbitrary \( S^z \). As a consequence, the subspace under the Tr in the last relations from Eqs. (13, 14) means that the trace should be taken only over the \( \mathcal{H}^{S^z} \) subspace.

For finite lattices the Tr operation means a finite sum which can be interchanged with the sum arising from the series expansion of the exponential function. We need in this case for calculations \( \text{Tr}_{\mathcal{H}^{S^z}} (\hat{H}_{\infty})^l \). This trace can be computed starting from Eqs. (13, 14). We have

\[
\text{Tr}_{\mathcal{H}^{S^z}} (\hat{H}_{\infty})^l = \sum_{P} \sum_{R} \sum_{i_1} \ldots \sum_{i_l} t_{i_1j_1} \ldots t_{i_lj_l} \times
\langle R | \hat{H}_{\infty}^{ij} | R_{l-1} \rangle \ldots \langle R_1 | \hat{H}_{\infty}^{ij} | \mathcal{R} \rangle \times
\langle \mathcal{P} | T^{S^z} \mathcal{C}(R_{l-1}; i_l, j_l) \ldots T^{S^z} \mathcal{C}(R_1; i_2, j_2) \ldots T^{S^z} \mathcal{C}(R; i_1, j_1) | \mathcal{P} \rangle.
\] (15)

Let us denote for \( \gamma(l) = \gamma(0) \) by \( \gamma \equiv (\gamma(0), \gamma(1), \ldots, \gamma(l-1), \gamma(l)) = (R, \mathcal{R}_1, \ldots, \mathcal{R}_{l-1}, \mathcal{R}) \) a sequence of \( \mathcal{R} \) permutations for which \( \prod_{i=1}^{l} \langle \gamma(i) | \hat{H}_{\infty} | \gamma(i-1) \rangle \neq 0 \). We call \( L(\gamma) : = l \) the length of \( \gamma \). The set of all the \( \gamma \)'s with length \( l \) will be denoted by \( \Omega_l \). Let consider now the lattice \( \Lambda_h \) consisting of every different hole configuration \( \mathcal{R} \). We recall that \( \mathcal{R} \) can be described by the ordered position of holes: \( (h_1 < \ldots < h_{N_h}) \). We consider two lattice points \( \mathcal{R} \) and \( \mathcal{R}' \) nearest neighbours if they differ by only one hole position, and these different hole positions are nearest neighbours in the original lattice \( \Lambda \). The lattice that we obtain in a such a way is a part of the \( D N_h \) dimensional hypercubic lattice, and \( \gamma \) is a sequence of nearest neighbour lattice points in \( \Lambda_h \). Because of this reason, we call \( \gamma \) a ,,loop”. In \( N_h = 1 \) case \( \gamma \) is a loop in the original lattice \( \Lambda \).

In the case of \( \sum_{i,j} t_{ij} \langle \mathcal{R}' | \hat{H}_{\infty}^{ij} | \mathcal{R} \rangle \neq 0 \) there is precisely one nearest neighbour pair \( \langle i, j \rangle \) for which \( \langle \mathcal{R}' | \hat{H}_{\infty}^{ij} | \mathcal{R} \rangle \neq 0 \). Therefore the loop \( \gamma \) uniquely determines a sequence of pairs of nearest neighbour indices \( \langle i_1, j_1 \rangle, \ldots, \langle i_l, j_l \rangle \) which gives the only one nonzero contribution of the sums \( \sum_{i_1, j_1} \ldots \sum_{i_l, j_l} \) in Eq. (13). Denoting the product of permutations
\( \mathcal{C}(\mathcal{R}; i, j) \) obtained from this nonzero term by \( \mathcal{P}_\gamma \), we have

\[
\text{Tr}_{\mathcal{H}_z} (\hat{H}_\infty)^l = \sum_{\gamma \in \Omega_l} \sum_{\mathcal{P}} \langle \mathcal{P} | T^{S_z}[\mathcal{P}_\gamma] | \mathcal{P} \rangle = \sum_{\gamma \in \Omega_l} \chi^{S_z}(\mathcal{P}_\gamma). \tag{16}
\]

As can be seen from Eq.(16) we obtain a sum of characters of \( T^{S_z}[\mathcal{P}_\gamma] \). Every character is constant on an arbitrary conjugate class \( C \). Therefore, the above character sum has \( N(C)(l) \) identical members, where \( N(C)(l) \) represents the number of the loops with length \( l \) for which \( \mathcal{P}_\gamma \in C \).

Using the notation \( \beta \) for \( t \)-times the reciprocal temperatures and the results for the sum of the characters \( \chi^{S_z} \) from Eqs.(26-27) from the Appendix, we obtain

\[
\langle \hat{S}^2 \rangle = \frac{3}{4Z} \sum_{l=0}^{\infty} \frac{\beta^l}{l!} \sum_{C \subset S_N} N^{(C)}(l) (-1)^{|C|} \left( 2\sum_{i=1}^{N} C_i \right) \left( \sum_{i=1}^{N} i^2 C_i \right), \tag{17}
\]

where, for the partition function we have

\[
Z = \sum_{l=0}^{\infty} \frac{\beta^l}{l!} \sum_{C \subset S_N} N^{(C)}(l) (-1)^{|C|} \left( 2\sum_{i=1}^{N} C_i \right). \tag{18}
\]

Here \( |C| \) is the parity of permutations from the conjugate class \( C \) and \( (C_1, C_2, \ldots, C_N) \) describes their cycle structure, i.e. these permutations contains \( C_i \) cycles with length \( i \).

Concerning the technical aspects in using Eq.(18) or Eq.(17) in concrete applications we mention that in order to deduce the coefficients \( N^{(C)}(l) \) one should follow the following procedure. We need to deduce a concrete \( \sum_{C \subset S_N} \) contribution at a fixed \( l \) value. For this:

1.) Start from a fixed hole configuration \( \mathcal{R}_1 \), and denote with different numbers every site occupied by electrons. 2.) A single step for a given hole it means that we have to interchange the given hole with a nearest neighbour number. 3.) Take \( l \) steps with the holes in such a way, that finally get back the original hole configuration (this is a loop with length \( l \)). In this process an arbitrary hole can be moved in every step, the order of the steps being relevant. However, by interchanging holes between them, we do not obtain new loops. 4.) Determine the cycle structure \( C \) of the permutation of the numbers for the obtained loop (i.e. obtain the numbers \( C_i \)). As a result of this analyses, we have find in this first step \( m = 1 \) one loop of length \( l \) and a given cycle structure \( \{C_i\}_{m=1} \). 5.) Go back to the step 3). and find a different loop with the same length \( l \) based on the same starting hole configuration \( \mathcal{R}_1 \).
After this step \( m = 2 \), we have another loop with length \( l \), and another cycle structure \( \{ C_i \}_{m=2} \).

6) If you have taken into account every possible different loop starting from the hole configuration \( R_1 \), do the same procedure with every possible different starting hole configuration \( R_j \).

7) All this being done, the summation \( \sum_{C \in S_N} \) at a fixed \( l \) means in fact a summation over all possible cycle structures obtained above. For example, given a concrete cycle structure \( \{ C_i \}_m = (C_1 = a_1, C_2 = a_2, ..., C_r = a_r) \) we may express with it \( \sum_i C_i \) or \( \sum_i i^2 C_i \), the quantity \( N^{(C)}(l) \) having the meaning of how many times this concrete \( \{ C_i \}_m \) cycle structure has been obtained in the procedure presented above. The number \( |C| \) gives the parity of all permutations which give the same cycle structure \( \{ C_i \}_m \) (as presented in the Appendix, all different permutations with the same cycle structure have the same parity).

8) As presented in the step 7), we have to sum over all possible cycle structures obtained in points 1)-6).

Using this procedure, with a computer, a partition function or a spin-square \( T \neq 0 \) expectation value can be deduced for a system with arbitrary number of holes. Evidently, the calculation time increases with the size of the systems, or number of holes.

**B. The free energy and specific heat**

> From the partition function \( Z \) given in Eq.(18) we can compute the free energy \( F = -T \ln Z \) and the specific heat \( c = T \frac{\partial^2 (T \ln Z)}{\partial T^2} \).

From Eq.(17) we correctly obtain paramagnetic behaviour at high temperatures in thermodynamic limit. The first term of the \( l \)-sum becomes dominant if \( T \) increases, and \( N^{(C)}(0) = 1 \) if \( C = 1 \) otherwise \( N^{(C)}(0) = 0 \). Therefore we have in high temperatures limit \( \langle \hat{S}^2 \rangle = 3N/4 \), so the value of the total spin per particle is proportional with \( 1/\sqrt{N} \).

In order to analyze the temperature dependence of \( \langle \hat{S}^2 \rangle \) we need the values of \( N^{(C)}(l) \) as functions of \( l \). Comparing Eq.(18) with the formula for the partition function \( Z \) derived in first quantized formalism we obtain
\[
\lim_{T \to 0} \sum_{l=0}^{\infty} \left( \frac{t}{\pi T} \right)^l \frac{1}{l!} N(C)(l) e^{-\frac{E_0}{k T}} = \frac{|C|}{N!}
\]

for arbitrary conjugate class \(C\) which can occur in Eqs. (17,18), where \(E_0\) is the ground state energy of the \(N\) particle hard core boson system.

### C. The Nagaoka state

The knowledge of the asymptotic behaviour given by the Eq. (19) is enough to analyze the \(T\) dependence of the Nagaoka ferromagnetism (i.e. \(N_h = 1\) case). In this situation \(\Omega_l\) contains the \(l\) length loops of the lattice \(\Lambda\). For one hole, \(R\) is uniquely determined by the position of the hole. The positions of the hole is described by \(\gamma(0)\) at the starting point of the loop, and \(\gamma(l) = P^{i_1,j_1} \ldots P^{i_l,j_l} \gamma(0) P^{-1}\) at the ending point of the loop are the same. It can be seen that the parity of \(|P| = (-1)^l\) is always even when we use open boundary conditions, because there is no loop with odd length in this case. It means that the dynamical evolution controlled by the Hamiltonian Eq. (1) is not able to permute the particles by odd permutations, given by the presence of the hard core potential acting between them. As a consequence, the fermionic character of the particles has absolutely no effect in this case. This is fully consistent with our previous statement (presented before Eq. (12) ) that the \(S = S_{max}\) spectrum of our original fermion system is equivalent with the spectrum of a hard core spinless boson system. Moreover, if bosons „existed” with half spin, then there would not be differences between the system consisting of these particles with hard core potential on a square lattice and our original fermionic system in the one hole case, because the permutations \(C(R_l ; i, j)\) occur in the Schrödinger equation Eq. (10) are always even, and for even permutations there are no difference between the representations \(T_S\) connected to bosons and fermions. As we mentioned above, the ground state wave function of a boson system is always symmetric, therefore the spin wave function is also symmetric, i.e. the ground state is ferromagnetic. This extreme ”symmetry” is an interesting explanation of Nagaoka’s theorem. Our formalism certainly gives back this result. It is obtained by taking
the $T \to 0$ limit in Eq.(17), considering the asymptotic behaviour of the coefficients $N^{(C)}(l)$
given by Eq.(19) for the conjugate classes with even parity and $N^{(C)}(l) = 0$ for odd parity,
furthermore using the result Eq.(25) from the Appendix. When we use periodic boundary
conditions we still have $|P \gamma| = (-1)^{L(\gamma)}$ which, however, can be odd, but only in the case
when the linear length of the lattice is odd at least in one direction, and $\gamma$ goes through the
boundary in this direction. In $t < 0$ case $\beta t(-1)^{|C|}$ is always positive, the sign coming from
the odd parity of the permutation is compensated by the sign obtained during the movement
around odd steps, therefore the above argumentation remains valid. The key feature now is
the fact, that the parity of $P \gamma$ is in one to one correspondence with the parity of $L(\gamma)$.

D. Cases with more than one hole

The existence of more than one hole permits arbitrary (even and odd) permutations
of the particles under the dynamical evolution (independently of the length of the loop),
therefore the fermionic feature of them play an important role in building up the energy
spectrum of the system. Using the asymptotic behaviour of $N^{(C)}(l)$ from Eq.(19) and the
results of the Appendix presented after Eq.(25), the $\langle S^2 \rangle$ value remains undetermined (i.e.
0/0), which is due in our interpretation to the fact that $E_0$ is not a possible energy for the
fermionic system any longer. The special similarity between bosons and fermions does not
remain valid, therefore we can not draw conclusion for the magnetic property of the system
based on Nagaoka’s theorem. There is a qualitative difference between the one and two
hole case. It is similar with the case when in a special point the Hamiltonian has an extra
symmetry, but the features of the model could be very different even close to this point
due to the symmetry breaking. If bosons would have half spin, a system consisting of such
hard core bosons on a lattice would be ferromagnetic even for arbitrary hole concentration.
This statement remains valid for real bosons with integer (non zero) spin as well and the
expectational value of the total spin goes to a macroscopical (but not to the maximum)
value when the temperature goes to zero, in this case.
In order to obtain information about the two (or more) hole case, the study of Eq.(17) is needed. To deduce the $N^C(l)$ numbers one can use Monte Carlo methods. For example, by random sampling we can determine the percentage of the contribution of loops with a given length in $P_\gamma \in C$. However, we have to mention, that the trace over the spin degrees of freedom has been taken already, and because of this reason, the presented procedure increases the efficiency of the usual world line algorithm. In this case, we need only a sampling from the world lines of the holes, which are $2^N$ times less than all the different world lines of the electrons. To see the trend of the magnetic behaviour in the $T$ dependence, we have determined the $N^C(l)$ coefficients up to the 14-th order exactly, and further, from 15-th up to the 50-th order by Monte Carlo in the case of a $5 \times 5$ lattice with two holes. The square of the total spin per particle and the specific heat deduced from these results are presented in Fig1.a. and b. As the temperature decreases the error of our results increases, but it is clear that the total spin increases, which underline a tendency to ferromagnetism at $T \to 0$ within the accuracy of our calculation.

VII. SUMMARY

Summarizing, we have analyzed a simple one-band Hubbard model in $U = \infty$ limit in any dimensions. We have treated this problem for the case in which an arbitrary but fixed hole concentration is present within the system. Concentrating on the effect of the Hamiltonian on the charge and spin degrees of freedom and based on the representations of the symmetric group, we presented an exact Schrödinger equation in a form which explicitly shows the effect of the spin background in the movement of the holes. Explications related to the application of the presented equation in concrete situations were given in detail. Based on the deduced results we have showed that the effect of the spin background on the movement of holes is unimportant a) when the system is one dimensional with open boundary condition and b) in any dimensions when the spin of the background is maximum. In the first case the holes move as hard core spinless bosons, in the second case as hard core
spinless fermions. When we have $D > 1$ and $S \neq S_{\text{max}}$ the effect of the spin background seen in the motion of the holes and the energy spectrum is highly non-trivial. The Nagaoka ferromagnetism ($N_h = 1$ case) in our formalism is due to the fact that in the one hole case and $U = \infty$, the rearrangement of particles with odd parity permutations in the dynamical evolution of the system is impossible. Therefore, the fermionic feature is not playing any role, and the system is equivalent with a system of hypothetical hard core half-spin boson system whose ground state is trivially ferromagnetic. In the presence of more than one hole this is no more true and the complete separation of charge and spin degrees of freedom is impossible.

On the other hand, based on our representation of the Hamiltonian, the trace over the spin degrees of freedom can be computed exactly. The presented procedure allows us to express the partition function, free energy, specific heat and the expectational value of the square of the total spin. The calculations can be given based on the counting of loop contributions, whose steps were described in extreme details for potential applications. In principle the method allows to calculate $T \neq 0$ expectation values for an arbitrary number of holes, based on clear formal steps handable by computer. In the frame of this formalism the efficiency of the usual Monte Carlo methods can also be increased.

**APPENDIX**

In this Appendix we are presenting mathematical details related to deduced formulas presented in the paper. For the beginning we are presenting an overview of notations and definitions used, then rather technical proofs follow. For more mathematical details connected to the deduction procedure we refer to Hamermesh 1962.

We treat a permutation of degree $N$ as a bijective function $P : \{1, \ldots, N\} \to \{1, \ldots, N\}$. The product of two permutations is defined by the standard composition of them as functions (from right to left): $(PQ)(i) := P(Q(i))$. The symmetric group of degree $N$ formed by all the permutations of degree $N$ is denoted by $S_N$. For $M \subset \{1, \ldots, N\}$ the group
$S_M$ formed by all the bijections from $M$ onto itself is a natural subgroup of $S_N$, a function of $S_M$ acts identically on the elements of $\{1, \ldots, N\} \setminus M$. We denote the transposition which interchanges $i$ and $j$ by $P^{(i,j)}$, and $C^{(i\rightarrow j)}$ the cycle which moves $i$ into $j$ while pushing left (right) the elements between $i$ and $j$ with $1$ if $i < j$ ($i > j$). The group algebra $C[S_N]$ is a complex Hilbert space generated by the elements of $S_N$ as an orthonormal basis. The associative but noncommutative product of two elements of the group algebra defined by the convolution:

$$ab \equiv \left( \sum_{P \in S_N} \alpha_P \ P \right) \left( \sum_{Q \in S_N} \beta_Q \ Q \right) = \sum_{P \in S_N} \sum_{Q \in S_N} \alpha_P \beta_Q \ P \ Q = \sum_{P \in S_N} \left( \sum_{Q \in S_N} \alpha_Q \beta_{Q^{-1} P} \right) P.$$

If a subalgebra $\mathfrak{I}$ has the property that, for $a$ in $\mathfrak{I}$, $ab$ is also in $\mathfrak{I}$ for any elements $b$ of the whole algebra, then $\mathfrak{I}$ is called a right ideal. If $e$ is an idempotent element of the algebra ($e \ e = e$) then $e \ C[S_N] = \{ e \ a \ | \ a \in C[S_N] \}$ is a right ideal, because of the associativity of the group algebra. It remains true if $e$ is only essentially idempotent ($e \ e = c \ e$, $c \in C$) because $e' = e / c$ is idempotent.

Now we verify that the Hilbert space generated by all the vectors $|R, \ P\rangle$ with arbitrary but fixed $R$ is isomorphic with a proper right ideal of the group algebra $C[S_N]$. (In the following $N$ and $S^z$ are fixed.) We recall that for fixed $S^z$ we denote by $\sigma$ the following function: $\sigma(i) := \uparrow$ if $i \in \{1, \ldots, N_\uparrow = N/2 + S^z\}$ and $\sigma(i) := \downarrow$ if $i \in \{N_\downarrow + 1, \ldots, N\}$. Let’s denote the subgroup of $S_N$ the elements of which permute the numbers of the set $\sigma^{-1}(\uparrow)$ by $K_\uparrow = S_{\sigma^{-1}(\uparrow)}$. Similarly, the permutations of $K_\downarrow = S_{\sigma^{-1}(\downarrow)}$ permute only the $\sigma^{-1}(\downarrow)$ numbers. Let $K = K_\uparrow \times K_\downarrow$, the direct product of $K_\uparrow$ and $K_\downarrow$. It can be seen that

$$e^{S^z} := \frac{1}{\sqrt{|K|}} \sum_{P \in K} P \quad (20)$$

is essentially idempotent, ($|K| = N_\uparrow! \ N_\downarrow!$ is the order of the subgroup $K$) therefore $\mathfrak{I}^{S^z} := e^{S^z} \ C[S_N]$ is a right ideal. For different permutations $P$ and $Q$ the elements $e^{S^z} P$ and $e^{S^z} Q$ of the ideal $\mathfrak{I}^{S^z}$ are the same if and only if the permutations are in the same right coset with respect to the subgroup $K$ (i.e. $P = P' \ Q$, $P' \in K$), because in the expression
\[ \sum_{P \in K} P P' Q = \sum_{P' \in K} P'' Q = \sum_{Q' \in K} Q' \] the sum is taken over the right coset \( K \), and they form a disjoint cover of the group.

Examining the basis vectors \(| \mathcal{R}, \mathcal{P} \rangle\) for a fixed \( \mathcal{R} \) can be seen that the definition Eq.(5) gives the same vector for different permutations \( \mathcal{P} \) and \( \mathcal{P}' \mathcal{P} (\mathcal{P}' \in K) \) from the same right coset, because \( \sigma(\mathcal{P}(i)) = \sigma(\mathcal{P}'\mathcal{P}(i)), \ (i \in \{1, \ldots, N\}) \). However, permutations \( \mathcal{P}_1 \) and \( \mathcal{P}_2 \) from different right cosets mix the numbers \( \sigma^{-1}(\uparrow) \) and \( \sigma^{-1}(\downarrow) \) with each other differently, therefore they lead to different spin configurations.

The above two paragraphs prove that the map \(| \mathcal{R}, \mathcal{P} \rangle \rightarrow e^{Sz} \mathcal{P} \) for fixed \( \mathcal{R} \) is well-defined and injective. Let’s extend this map linearly over the whole space generated by the vectors \(| \mathcal{R} \rangle \otimes | \mathcal{P} \rangle\) with fixed \( \mathcal{R} \). Certainly we get a surjective map onto \( \mathbb{I}^{Sz} \), since the elements \( e^{Sz} \mathcal{P} \) generate this ideal. Now we show that this linear isomorphism also preserves the inner product. In the proof we denote the inner product in the group algebra by \((\ .\ ,\ .\ )\).

\[
( e^{Sz} \mathcal{P}, e^{Sz} \mathcal{Q} ) = \left( \frac{1}{\sqrt{|K|}} \sum_{s_1 \in K} S_1 \mathcal{P}, \frac{1}{\sqrt{|K|}} \sum_{s_2 \in K} S_2 \mathcal{Q} \right) = \frac{1}{|K|} \sum_{\mathcal{P}' \in K \mathcal{P}} \sum_{\mathcal{Q}' \in K \mathcal{Q}} (\mathcal{P}', \mathcal{Q}') . \tag{21}
\]

If the right cosets \( K \mathcal{P} \) and \( K \mathcal{Q} \) are different then they have no common elements, therefore \( (\mathcal{P}', \mathcal{Q}') = 0 \). (The elements \( \mathcal{P} \in S_N \) are orthonormals by definition.) If the right cosets \( K \mathcal{P} \) and \( K \mathcal{Q} \) are the same then the sums have \( |K| \) different members which give 1 (in case \( \mathcal{P}' = \mathcal{Q}' \)), the rest are zero, so the final result is 1.

We showed that the Hilbert spaces generated by the vectors \(| \mathcal{R}, \mathcal{P} \rangle\) with arbitrary but fixed \( \mathcal{R} \) are isomorphic with \( \mathbb{I}^{Sz} \) therefore also with each other. This space is denoted by \( \mathcal{H}^{Sz} \) instead of \( \mathbb{I}^{Sz} \). The image of \(| \mathcal{R}, \mathcal{P} \rangle\) by this isomorphism is independent of \( \mathcal{R} \). This element of \( \mathcal{H}^{Sz} \) is denoted by \(| \mathcal{P} \rangle\). Based on the above defined Hilbert space isomorphism we identify \( \mathcal{H}^{Sz} \) with \( \mathbb{I}^{Sz} \) and we distinct neither the notations of the inner product nor the operators act on them anymore. We can regard a linear operator defined on \( \mathbb{I}^{Sz} \) as an operator on \( \mathcal{H}^{Sz} \) and vice versa.

Similar technical and even more simpler work to prove that the space \( \mathcal{H}_c \) is isomorphic with the Hilbert space of the system of \( N \) (or equivalently \( N_h \)) hard core spinless particles,
and its basis characterized by the positions of these particles uniquely determines the basis vector \(| \mathcal{R} \rangle \).

The formula

\[
T[Q]P := (-1)^{|Q|} P Q^{-1}
\]

defines a representation of the symmetric group in the group algebra. Here \(T[Q]\) is a linear operator associated with \(Q \in S_N\) by the representation \(T\), and \(P\) is a vector as an element of \(C[S_N]\). This representation is fully reducible. It is clear from the definition that every right ideal is an invariant subspace of this representation, thus \(T^{S_z} := T|_{\mathbb{S}^{S_z}}\) is also a representation (with lower dimension) of the symmetric group in \(\mathbb{S}^{S_z}\). Comparing the above defined representation and the effect of the Hamiltonian on a basis vector \(| \mathcal{R} \rangle \otimes | P \rangle\) as can be seen from Eq. (8), it is clear that the effect on the spin configuration can be described by the operator \(T^{S_z}[C(\mathcal{R}; i, j)]\), and we get Eq. (9).

Now we compute the character of the representation \(T^{S_z}\). By definition the character is the trace of the operator \(T^{S_z}[P]\) for a \(P \in S_N\).

\[
\chi^{S_z}(P) = \sum_{|Q|} \langle Q | T^{S_z}[P] | Q \rangle = \frac{1}{|K|} \sum_{Q \in S_N} \langle e^{S_z} Q | T^{S_z}[P] | e^{S_z} Q \rangle
\]

\[
= \frac{1}{|K|} \sum_{Q \in S_N} \langle e^{S_z} Q | (-1)^{|P|} e^{S_z} Q P^{-1} \rangle = \frac{(-1)^{|P|}}{|K|^2} \sum_{Q \in S_N} \sum_{S_1, S_2 \in K} \langle S_1 Q | S_2 Q P^{-1} \rangle
\]

\[
= \frac{(-1)^{|P|}}{|K|^2} \sum_{Q \in S_N} \sum_{S_1, S_2 \in K} \delta_{S_1 Q, S_2 Q P^{-1}} = \frac{(-1)^{|P|}}{|K|} \sum_{Q \in S_N} \sum_{S \in K} \delta_{QP Q^{-1}, S}.
\] (23)

Every element \(P'\) of the conjugate class \(C^P\) which contains \(P\) appears as \(Q P Q^{-1}\) the same times. That’s why there are \(|S_N| / |C^P|\) permutations \(Q\) for which \(QP Q^{-1} = P'\). (\(|X|\) means the number of the elements of the set \(X\).) If \(P'\) is in \(K\) then the second sum in the last row of Eq. (23) has one non-zero element, otherwise it does not. Therefore the character

\[
\chi^{S_z}(P) = (-1)^{|P|} \frac{|S_N| |C^P \cap K|}{|K| |C^P|}
\]

\[
= (-1)^{|P|} \frac{C_1^P}{c_1^P \cdot c_1'} \cdot \frac{C_2^P}{c_2^P \cdot c_2'} \cdot \ldots \cdot \frac{C_N^P}{c_N^P \cdot c_N'}
\]
\[ = (-1)^{|\mathcal{P}|} \sum_{c_1, \ldots, c_N} \prod_{i=1}^{N} \binom{C_i^P}{c_i}, \quad (24) \]  

where the cycle structure of every elements of the conjugate class \( C^P \) is described by the \( N \) pieces of numbers \( C_1^P, C_2^P, \ldots, C_N^P \) by the following way: these permutations contains \( C_1^P \) cycles with length 1, \( C_2^P \) cycles with length 2, etc. For the second equality see Hamermesh 1962, the third can be obtained with simple computation.

We need the sum of these characters on an arbitrary conjugate class \( C \subset A_N \) where \( A_N \) is the alternating group formed by all the even permutations of \( S_N \). Based on the first line of the formula Eq.(24) we can see, that

\[
\sum_{C \subset A_N} |C| \chi_S^z(C) = \frac{N!}{|K_S^z|} |A_N \cap K_S^z| = \frac{N!}{2}.
\]  

(25)

The similar sum over the conjugate class which has no common element with \( A_N \) gives the result \(- N! / 2\). The even permutations form an invariant subgroup in \( S_N \) therefore every conjugate class is in \( A_N \) or disjoint from it. Hence \( \sum_{C \subset S_N} |C| \chi_S^z(C) = 0 \).

Based on the last line of the formula Eq.(24) we can get:

\[
\sum_{S^z=-N/2}^{N/2} \chi_S^z(C) = (-1)^{|C|} 2 \sum_{i=1}^{N} c_i.
\]  

(26)

Furthermore

\[
\sum_{S^z=-N/2}^{N/2} (S^z)^2 \chi_S^z(C) = (-1)^{|C|} 2 \sum_{i=1}^{N} c_i \left( \frac{1}{4} \sum_{i=1}^{N} i^2 c_i \right).
\]  

(27)

The representation \( T^{S^z} \) is not irreducible if \( S^z \neq S^z_{\max} \) or \( S^z_{\min} \). Certainly it can be verified in pure mathematical way, but physically it is due to the SU(2) rotational symmetry in the spin space. The operator \( \hat{S}^- \) realizes a linear bijection between the spaces \( \mathcal{H}^{S^z,S}_{s} \) and \( \mathcal{H}^{S^z-1,S}_{s} \) if \( S \geq S^z \). Moreover \([\hat{H}_\infty, \hat{S}^-]=0\), therefore the effect of the Hamiltonian is equivalent on the space \( \mathcal{H}^{S^z,S}_{s} \) and \( \mathcal{H}^{S^z-1,S}_{s} \). The effect of the Hamiltonian on the space \( \mathcal{H}^{S^z}_{s,\max} = \mathcal{H}^{S^z_{\max},S^z_{\max}}_{s} \) can be described by the representation \( T^{S^z}_{s,\max} = T^{S^z}_{s,\max}, \) hence it is true for the space \( \mathcal{H}^{S^z_{\max}-1,S^z_{\max}}_{s} \). However, the effect of the Hamiltonian on \( \mathcal{H}^{S^z}_{s,\max}-1 \) is described by the representation \( T^{S^z}_{s,\max}-1 \), which according to the above coincides with
\( T_{S_{max}} \) on \( \mathcal{H}^S_{S_{max-1},S_{max}} \) which is therefore an invariant subspace. Therefore \( T^S_{S_{max-1}} \) is not irreducible therefore it is fully reducible (because it is a finite dimensional representation of a finite group). Therefore the orthogonal complementer of \( \mathcal{H}^S_{S_{max-1},S_{max}} \) which is the \( \mathcal{H}^S_{S_{max-1},S_{max-1}} \) is also an invariant subspace. The restriction of \( T^S_{S_{max-1}} \) to this subspace we denote by \( T_{S_{max-1}} := T^S_{S_{max-1}} \mid \mathcal{H}^S_{S_{max-1},S_{max-1}} \). Continuing this process on this line, acting by \( \hat{S}^- \) again and again, we get: \( T^{S_z} \cong \bigoplus_{S=|S_z|}^{N/2} T_S \).

In other words this means that the functions \( \varphi^{S_z,S}_s \), which describe the spin configuration with \( S \) and \( S^z \) values of the total spin and its \( z \) component for fixed hole configuration, form a space of a representation of the symmetric group. This above defined representation depending only on the value of \( S \) was denoted by \( T_S \), and the effect of the Hamiltonian on the spin configuration can be described by this representation:

\[
\hat{H}_{ij} \mid \varphi^{S_z,S}_s \rangle = T_S[ \mathcal{C}(\mathcal{R}; i, j) ] \mid \varphi^{S_z,S}_s \rangle \quad (28)
\]

The matrices of the representations \( T_S \) can be given by algebraic methods, see e.g. Hamermesh 1962. These methods are usable only in case of few particles. In this case we can use the expression Eq.(10) to get exact diagonalization results.

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FIG. 1. The a: square of the total spin and b: specific heat as a function of the reduced temperature in the case of $5 \times 5$ lattice with two holes. The calculation based on the Eqs. 17-18 in which the coefficients $N^{(C)}(l)$ are taken into account exactly up to $l = 14$ and determined by Monte Carlo simulation up to $l = 50$. 