Antiferromagnetism of the 2D Hubbard Model at Half Filling: Analytic Ground State at Weak Coupling

Michele Cini and Gianluca Stefanucci

Istituto Nazionale di Fisica della Materia, Dipartimento di Fisica,
Universita’ di Roma Tor Vergata, Via della Ricerca Scientifica, I-00133
Roma, Italy

We introduce a local formalism to deal with the Hubbard model on a \( N \times N \) square lattice (for even \( N \)) in terms of eigenstates of number operators, having well defined point symmetry. For \( U \to 0 \), the low lying shells of the kinetic energy are filled in the ground state. At half filling, using the \( 2N - 2 \) one-body states of the partially occupied shell \( S_{hf} \), we build a set of \( \left( \frac{2N - 2}{N - 1} \right)^2 \) degenerate unperturbed ground states with \( S_z = 0 \) which are then resolved by the Hubbard interaction \( \hat{W} = U \sum \hat{n}_{r \uparrow} \hat{n}_{r \downarrow} \). In \( S_{hf} \) we study the many-body eigenstates of the kinetic energy with vanishing eigenvalue of the Hubbard repulsion (\( W = 0 \) states). In the \( S_1 = 0 \) sector, this is a \( N \) times degenerate multiplet. From the singlet component one obtains the ground state of the Hubbard model for \( U = 0^+ \), which is unique in agreement with a theorem by Lieb.

The discovery of high temperature superconductors \(^1\) enhanced the interest in models of two-dimensional, strongly correlated electron systems, such as the 2D Hubbard model. The (repulsive) Hubbard hamiltonian is highly idealised, for instance two particles are allowed to interact only on-site, yet the model already displays an interesting phase diagram. The fluctuation exchange (FLEX) \(^2\) diagrammatic approach, which is based on a conserving approximation and, independently, renormalization group techniques \(^3\) \(^4\) show that near the antiferromagnetic phase at half filling, there exists a superconducting phase too, with a momentum dependent gap, of \( d \) wave symmetry. Indication of a possible instability of the Fermi liquid towards pairing near half filling also comes from cluster diagonalizations \(^5\) \(^6\) \(^7\). Therefore, exact results on the half filled Hubbard model may be relevant to antiferromagnetism and to the mechanism of the superconducting instability as well.

In the strong coupling limit the double occupation of the same site is energetically suppressed and the model at half filling is equivalent to the Heisenberg model with an antiferromagnetic exchange interaction \(^8\). A popular approach takes care of the strong repulsion between two opposite spin fermions by a Gutzwiller \(^9\) projection, i.e. by throwing out of the Hilbert space the double occupation states.

However, truncating the Hilbert space in this way costs lots of kinetic energy, so at finite \( U \) the system must allow double occupation, also in the ground state. At weak coupling it makes sense to speak about particles in filled shells, which behave much as core electrons in atomic physics, and particles in partially filled, or valence, shells. Remarkably, particles in partially filled shells can totally avoid double occupation at no cost in energy: they do so, forming \( W=0 \) states, that are defined as many-particle eigenstates of the kinetic energy with no double occupation. Below, using a new formalism, we show how \( W = 0 \) states arise by symmetry.

An important theorem on the Hubbard model at half filling is due to Lieb \(^10\): the ground state for a bipartite lattice is unique and has spin \( \frac{1}{2} |S_1| - |S_2| \) where \( |S_1| \) (\( |S_2| \)) is the number of sites in the \( S_1 \) (\( S_2 \)) sublattice; here and in the following, \( |S| \) will be the number of elements in the set \( S \). It is worth to observe that the theorem makes no assumptions about the symmetry of the lattice. For a \( N \times N \) square lattice, with \( N \) even, the ground state is a singlet and in Ref. \(^11\) it was shown that in the strong coupling limit it has total momentum \( K_{tot} = (0, 0) \) and \( s \) wave \( (x^2 + y^2) \) or \( d \) wave \( (x^2 - y^2) \) symmetry for even or odd \( N/2 \) respectively.

In this paper we build the exact ground state of the Hubbard model at half filling and weak coupling. In Section \(^1\) we state more precisely the problem we want to solve and we define some notations. In
Section II we show how for each site we can build a local one-body basis set, which is well suited to write the antiferromagnetic many-body wave function. Finally in Section III we explore the symmetry properties of the ground state, and deduce the same quantum numbers as predicted by Refs. [10] [11] at strong coupling.

The present approach lends itself to obtain exact results for other fillings as well, but this will be shown elsewhere [2].

II. THE HUBBARD MODEL AT HALF FILLING AND WEAK COUPLING

Let us consider the Hubbard model with Hamiltonian

$$H = H_0 + \hat{W} = i \sum_{\langle r, r' \rangle} \sum_{\sigma} c_{r, \sigma}^\dagger c_{r', \sigma} + \sum_r U \hat{n}_{r, \uparrow} \hat{n}_{r, \downarrow}, \quad U > 0,$$

(1)

on a square lattice of $N \times N$ sites with periodic boundary conditions and even $N$. Here $\sigma = \uparrow, \downarrow$ is the spin and $r, r'$ the spatial degrees of freedom of the creation and annihilation operators $c^\dagger$ and $c$ respectively. The sum on $\langle r, r' \rangle$ is over the pairs of nearest neighbors sites and $\hat{n}_{r, \sigma}$ is the number operator on the site $r$ of spin $\sigma$. The point symmetry is $C_{4v}$, the Group of a square [13]; besides, $H$ is invariant under the commutative Group of Translations $T$ and hence the Space Group [14] $G = T \otimes C_{4v}$; $\otimes$ means the semidirect product. We represent sites by $r = (i_x, i_y)$ and wave vectors by $k = (k_x, k_y) = \frac{2\pi}{N}(i_x, i_y)$, with $i_x, i_y = 0, \ldots, N - 1$. In terms of the Fourier expanded fermion operators $c_{k, \sigma} = \frac{1}{N} \sum_r e^{i k r} c_{r, \sigma}$, we have $H_0 = \sum_k \epsilon(k) c_{k, \sigma}^\dagger c_{k, \sigma}$ with $\epsilon(k) = 2t(\cos k_x + \cos k_y)$. Then the one-body plane wave state $c_{k, \sigma}^\dagger |0\rangle \equiv |k\sigma\rangle$ is an eigenstate of $H_0$.

We study the ground state. Let $S_{hf}$ denote the set (or shell) of the $k$ wave vectors such that $\epsilon(k) = 0$. At half filling ($N^2/2$ particles) for $U = 0$ the $S_{hf}$ shell is half occupied, while all $|k\rangle$ orbitals such that $\epsilon(k) < 0$ are filled. The $k$ vectors of $S_{hf}$ lie on the square having vertices $(\pm \pi, 0)$ and $(0, \pm \pi)$; one readily realizes that the dimension of the set $S_{hf}$, is $|S_{hf}| = 2N - 2$. Since $N$ is even and $H$ commutes with the total spin operators,

$$\hat{S}_z = \frac{1}{2} \sum_r (\hat{n}_{r, \uparrow} - \hat{n}_{r, \downarrow}), \quad \hat{S}^+ = \sum_r c_{r, \uparrow}^\dagger c_{r, \downarrow}, \quad \hat{S}^- = (\hat{S}^+)^\dagger,$$

(2)

at half filling every ground state of $H_0$ is represented in the $S_z = 0$ subspace. Thus, $H_0$ has $\binom{2N - 2}{N - 1}^2$ degenerate unperturbed ground state configurations with $S_z = 0$. We wish to study below how this degeneracy is removed by the Coulomb interaction $\hat{W}$ already in first-order perturbation theory. Actually most of the degeneracy is removed in first-order, and with the help of Lieb’s theorem we shall be able to single out the true, unique ground state of $H$. In Appendix A we show that the structure of the first-order wave functions is gained by diagonalizing $\hat{W}$ in the truncated Hilbert space $\mathcal{H}$ spanned by the states of $N - 1$ holes of each spin in $S_{hf}$. In other terms, one solves a $2N - 2$-particle problem in the truncated Hilbert space $\mathcal{H}$ and then, understanding the particles in the filled shells, obtains the first-order eigenfunctions of $H$ in the full $N^2$-particle problem. We underline that the matrix of $H_0$ in $\mathcal{H}$ is null, since by construction $\mathcal{H}$ is contained in the kernel of $H_0$.

The operator $\sum_r \hat{n}_{r, \uparrow} \hat{n}_{r, \downarrow}$ has eigenvalues $0, 1, 2, \ldots$ and so the lowest eigenvalue of $\hat{W}$ is zero (in other terms, $\hat{W}$ is positive semi-definite). The unique ground state of the Hubbard Hamiltonian for $U = 0^+$ at half filling will turn out to be a $W = 0$ singlet state of $2N - 2$ holes in $S_{hf}$ (filled shells being understood). We shall obtain the $W = 0$ states $\in \mathcal{H}$. It is clear that, although the $U = 0$ case is trivial, at $U = 0^+$ we are still facing a bona fide many-body problem, that we are solving exactly [15].

III. LOCAL FORMALISM FOR THE GROUND STATE WAVE FUNCTION

In the present section we first define a basis of local orbitals; then, we demonstrate a method for actually constructing the basis in the general case. We use the $4 \times 4$ case as a simple example
and then generalize. Then we show that using the local basis, the many body wave function of the antiferromagnetic ground state can be projected out as the singlet component of a single determinant, which is amazingly simple for an interacting system.

A. The Basis Set: Definition

Since \( \hat{W} \) depends on the occupation number operators \( \hat{n}_r \), it is intuitive that its properties in \( \mathcal{H} \) are best discussed by a suitable one-body basis of \( \mathcal{S}_{hf} \) such that at least one of these operators is diagonal. In addition, a convenient basis should exploit the large \( G \) symmetry of the system. If \( \mathcal{S}_{hf} \) were a complete set \( (N^2) \) states, one would trivially go from plane waves to atomic orbitals by a Fourier transformation; instead, we must define the local counterparts of plane-wave states using only the \( 2N - 2 \) states that belong to \( \mathcal{S}_{hf} \). For each site \( r \) we diagonalize the number operator \( \hat{n}_r \); moreover, since \( \hat{n}_r \) is compatible with the operations of the point symmetry group \( C_{4v} \) we also diagonalize the Dirac characters of the Group. The set of Dirac characters defines the irreducible representation \( \text{irrep} \); thus we write the one-body basis states \( \{ | \phi_\alpha^{(r)} \rangle \} \) where \( \alpha \) comprises the \( \hat{n}_r \) eigenvalue and a \( C_{4v} \) irrep label. However, different sites yield different sets; the eigenvectors \( | \phi_\alpha^{(0)} \rangle \) of \( n_{r=0} \) and those \( | \phi_\alpha^{(r)} \rangle \) of other sites \( r \) are connected by unitary transformations. Introducing the primitive translations of the lattice \( \hat{e}_x = (1,0) \) (one step towards the right) and \( \hat{e}_y = (0,1) \) (one step upwards) the primitive unitary transformations read:

\[
| \phi_\alpha^{(l,i)} \rangle = \sum_{\beta=1}^{2N-2} | \phi_\beta^{(0)} \rangle \langle \phi_\beta^{(0)} | \phi_\alpha^{(l,i)} \rangle = \sum_{\beta=1}^{2N-2} | \phi_\beta^{(0)} \rangle T_{\beta \alpha}^{(l)}, \quad l = x,y.
\]

The translation matrix \( T_l \) knows all the \( G \) symmetry of the system, and will turn out to be very special. Using such a basis set for the half filled shell the antiferromagnetic order of the ground state comes out in a clear and transparent manner.

B. Technique for Building the Basis Set

To accomplish that, it is not actually necessary to diagonalize any \( (2N - 2) \times (2N - 2) \) matrices. The number operator \( \hat{n}_r = c_r^\dagger c_r \) (for the moment we omit the spin index) is dealt with most easily by the following

**Theorem:** Let \( \mathcal{S} \) be an arbitrary set of plane-wave eigenstates \( \{ | k_i \rangle \} \) of \( H_0 \) and \( (n_r)_{ij} = \langle k_i | \hat{n}_r | k_j \rangle = \frac{1}{2\pi^2} e^{i (k_i - k_j) r} \) the matrix of \( \hat{n}_r \) in \( \mathcal{S} \). This matrix has eigenvalues \( \lambda_1 = \frac{|S|}{N^2} \) and \( \lambda_2 = \ldots = \lambda_{|S|} = 0 \).

Note that \( |S| \leq N^2 \); if \( |S| = N^2 \) the set is complete, like the set of all orbitals, and the theorem is trivial (a particle sitting on site \( r \) is the \( n_r \) eigenvector with eigenvalue 1); otherwise the theorem is an immediate consequence of the fact that (see Appendix B)

\[
\text{det}((n_r)_{ij} - \lambda \delta_{ij}) = (-\lambda)^{|S|-1} \left( \frac{|S|}{N^2} - \lambda \right), \quad \forall r.
\]

It is easy to verify that for \( r = 0 \) the eigenvector with nonzero eigenvalue is just the totally symmetric superposition of all the \( \{ | k_i \rangle \} \in S \).

Next, the large set \( \mathcal{S}_{hf} \) breaks into small pieces if we take full advantage of the \( G \) symmetry. Any plane-wave state \( k \) belongs to a one-dimensional irrep of \( T \); moreover, it also belongs to a star of \( k \) vectors connected by operations of \( C_{4v} \), and one member of the star has \( k_x \geq k_y \geq 0 \). We recall that any \( k \in \mathcal{S}_{hf} \) lies on a square with vertices on the axes at the Brillouin zone boundaries. Choosing an arbitrary \( k \in \mathcal{S}_{hf} \) with \( k_x \geq k_y \geq 0 \), hence \( k_x + k_y = \pi \), the set of vectors \( R_k \) is a basis for an irrep of \( G \). The high symmetry vectors \( k_A = (\pi,0) \) and \( k_B = (0,\pi) \) are the basis of the only two-dimensional irrep of \( G \), which exists for any \( N \). If \( N/2 \) is even, one also finds the high symmetry wavevectors \( k = (\pm \pi/2, \pm \pi/2) \) which mix among themselves and yield a four-dimensional irrep. In general, when \( k \) is not in a special symmetry direction, the vectors \( R_k \) are all different, so all the other irreps of \( G \) have dimension 8, the number of operations of the point Group \( C_{4v} \).
Below, we shall need the number of these irreps. Since 8 times the number of eight-dimensional irreps plus 4 times that of four-dimensional ones + 2 for the only two-dimensional irrep must yield $|S_{hf}| = 2N - 2$, one finds that $S_{hf}$ contains $N_e = \frac{1}{2}(N^2 - 2)$ irreps of dimension 8 if $N/2$ is even and $N_e = \frac{1}{2}(N^2 - 1)$ irreps of dimension 8 if $N/2$ is odd.

We note incidentally that $G$ cannot explain the degeneracy $2N - 2$ of $S_{hf}$, because the maximum dimension of its irreps is 8. Indeed, the accidental degeneracy of several irreps is due to the presence of extra symmetry, i.e. $G$ is a subgroup of the Optimal Group defined in Ref. [16].

In this way, $S_{hf}$ is seen to be the union of disjoint bases of different irreps of the Space Group. This break-up of $S_{hf}$ enables us to carry on the analysis and build the basis for any $N$. For illustration, we will first consider the case $N = 4$ and then generalize.

C. Example: Basis Set and Ground State for the $4 \times 4$ Square Lattice

As already noted, $k_A = (\pi, 0)$ and $k_B = (0, \pi)$ belong to $S_{hf}$ and are the basis of a two-dimensional irrep of $G$. The $2 \times 2$ matrix $(n_{\tau=0})_{ij} = \langle k_i | \tilde{n}_{\tau=0} | k_j \rangle$, with $i, j = A, B$, has the eigenvector $|\psi_{A1}^{(0)}\rangle = \frac{1}{\sqrt{2}}(|k_A\rangle + |k_B\rangle)$ with eigenvalue $\lambda_1 = 1/8$, in agreement with the above theorem. The second eigenvector, with vanishing eigenvalue, is $|\psi_{B1}^{(0)}\rangle = \frac{1}{\sqrt{2}}(|k_A\rangle - |k_B\rangle)$. As the notation implies, both are simultaneously eigenvectors of the Dirac characters and carry symmetry labels; actually the symmetries $A_1$ and $B_1$ could have been predicted without diagonalization because the two-dimensional irrep of $G$ breaks into $A_1 \oplus B_1$ in $C_{4v}$.

Translating by $r$, plane wave states pick up a phase factor: $|k\rangle \rightarrow e^{ikr}|k\rangle$. Thus, the eigenstates of $n_\tau$ are $|\psi_{A1}''(r)\rangle = \frac{1}{\sqrt{2}}(e^{ik_A} |k_A\rangle + e^{ik_B} |k_B\rangle)$ with $\lambda_1 = 1/8$ and $|\psi_{B1}''(r)\rangle = \frac{1}{\sqrt{2}}(e^{ik_A} |k_A\rangle - e^{ik_B} |k_B\rangle)$ with $\lambda_2 = 0$. The primitive translations (3) are performed by:

$$|\psi_{I}''(z)\rangle = \sum_{J=A_1,B_1} |\psi_{J}''(0)\rangle \langle \psi_{J}''(0) | \psi_{I}''(z)\rangle = \sum_{J=A_1,B_1} |\psi_{J}''(0)\rangle (T_{I})_{JJ}, \quad I = x, y$$

with $I = A_1, B_1$. Using eq. (3) one finds the antidiagonal translation matrices $T_I$

$$T_x = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, \quad T_y = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (6)$$

So, the orbital of $A_1$ symmetry at $r = 0$ has $B_1$ symmetry around the nearest neighbour sites, and conversely. In particular, $|\psi_{A1}''(0)\rangle$ has vanishing amplitude on a sublattice and $|\psi_{B1}''(0)\rangle$ on the other. The two-body state $|\psi_{A1}''(0)\rangle_{-\sigma} |\psi_{B1}''(0)\rangle_{-\sigma}$ has occupation for spin $\sigma$ but not for spin $-\sigma$ on the site $r = 0$; under a lattice step translation it flips the spin and picks up a (-1) phase factor:

$$|\psi_{A1}''(0)\rangle_{-\sigma} |\psi_{B1}''(0)\rangle_{-\sigma} \leftrightarrow |\psi_{B1}''(0)\rangle_{-\sigma} |\psi_{A1}''(0)\rangle_{-\sigma} = - |\psi_{A1}''(0)\rangle_{-\sigma} |\psi_{B1}''(0)\rangle_{-\sigma}; \quad (7)$$

therefore it has double occupation nowhere and is a $W = 0$ state (more precisely, a $W = 0$ pair [7] [8]).

For $N = 4$, $S_{hf}$ also comprises the basis $k_1 = (\pi/2, \pi/2)$, $k_2 = (-\pi/2, \pi/2)$, $k_3 = (\pi/2, -\pi/2)$, $k_4 = (-\pi/2, -\pi/2)$ of the 4-dimensional irrep of $G$. This irrep breaks into $A_1 \oplus B_2 \oplus E$ in $C_{4v}$, and such are the symmetry labels of the eigenvectors of $\tilde{n}_{\tau=0}$. We easily obtain them using the projection operators of $C_{4v}$. Letting $I = 1, 2, 3, 4$ for the irreps $A_1, B_2, E_x, E_y$ respectively, we can write down all the eigenvectors of $(k_i | \tilde{n}_{\tau=0} | k_j)$, with $i, j = 1, \ldots, 4$, as $|\psi_{I}^{(0)}\rangle = \sum_{i=1}^{4} O'_{I,i} |k_i\rangle$, where $O'$ is the following $4 \times 4$ orthogonal matrix

$$O' = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \end{bmatrix}. \quad (8)$$
The state with non-vanishing eigenvalue is again of $A_1$ symmetry. Translating by $r$ we readily get the eigenstates $|\psi^{(r)}_j\rangle$ of $n_r$ and of the Dirac characters; in this way, we calculate the translation matrices
\[ (T_{ij})_{JI} = \langle \psi^{(0)}_j | \psi^{(0)}_i \rangle \], which are block-antidiagonal:
\[ T_x = \begin{bmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{bmatrix}, \quad T_y = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}. \tag{9} \]

These $4 \times 4$ translation matrices are again very special; they are such that for each lattice step the subspace of $A_1$ and $B_2$ symmetry is mapped in the one spanned by $W$ and we are getting a new one for each irrep of $G$. The state with non-vanishing eigenvalue is again of $A_1$ symmetry. Translating by $r$ we readily get the eigenstates $|\psi^{(r)}_j\rangle$ of $n_r$ and of the Dirac characters; in this way, we calculate the translation matrices
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translation matrix \((T_i)_{ij} = \langle \phi_i^{(0)} | \phi_j^{(c_i)} \rangle\) is a block antidiagonal matrix:

\[
T_x = \begin{bmatrix}
0 & 0 & 0 & -\frac{1}{\sqrt{2}} & i\sqrt{\frac{3}{2}} & 0 \\
0 & 0 & 0 & -\frac{1}{\sqrt{2}} & -i\sqrt{\frac{3}{2}} & 0 \\
-\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\
i\sqrt{\frac{3}{2}} & -i\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 \\
0 & 0 & -i & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}, \quad T_y = \begin{bmatrix}
0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -i\sqrt{\frac{3}{2}} \\
0 & 0 & 0 & \frac{1}{\sqrt{2}} & i\sqrt{\frac{3}{2}} & 0 \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
i\sqrt{\frac{3}{2}} & i\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 \\
-i\sqrt{\frac{3}{2}} & -i\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0
\end{bmatrix}.
\] (13)

The \(|\varphi\rangle\) local basis at any site \(r\) splits into the subsets \(S_a = \{ |\varphi_1^{(r)}\rangle, |\varphi_2^{(r)}\rangle, |\varphi_3^{(r)}\rangle \}\), and \(S_b = \{ |\varphi_4^{(r)}\rangle, |\varphi_5^{(r)}\rangle, |\varphi_6^{(r)}\rangle \}\); a shift by a lattice step sends members of \(S_a\) into linear combinations of the members of \(S_b\), and conversely. For the present 4 × 4 case, we could have obtained the \(\varphi\) basis somewhat more simply by direct diagonalization on the whole set \(S_{hf}\), but the present approach has the advantage of being viable at large \(N\).

Indeed, \(|\varphi_1^{(0)}\varphi_2^{(0)}\rangle\) is equivalent to \(|\tilde{\psi}^{(0)}\varphi_1^{(0)}\rangle\), because this is just a unitary transformation of the \(A_1\) wave functions. Thus, we may write:

\[
|\Phi_{AF}\rangle^\sigma = |\varphi_1^{(0)}\varphi_2^{(0)}\varphi_3^{(0)}\varphi_4^{(0)}\varphi_5^{(0)}\varphi_6^{(0)}\rangle^\sigma.
\] (14)

Besides being useful for the sake of illustration because of its relative simplicity, the 4 × 4 case can be thoroughly explored on the computer, since the size of \(\mathcal{H}\) at half filling is 400. We have used Mathematica to diagonalize \(H + \xi S^2\), where a small \(\xi\) is a numerical device to keep the different spin components of the ground state separated. In this way, we observed the fourfold degenerate, \(W = 0\) ground state which \(\xi\) separates into its singlet, triplet, quintet and septet components, as expected, with the separation growing like \(U^2\). The antiferromagnetic property of the wave functions was also easily and nicely borne out by the numerical results.

**D. The \(N \times N\) Square Lattice for general Even \(N\)**

As discussed in Sect. III B, we break \(S_{hf}\) in the bases of irreps of \(G\) it contains. Each basis consists of plane-wave eigenstates \(|k_i\rangle\) of \(H_0\) and is converted in a local one-body basis at site \(r\) by diagonalizing \(n_r\) and Dirac’s characters. For \(N > 4\), \(S_{hf}\) contains \(k\) vectors that do not possess any special symmetry and we get eight-dimensional irreps of \(G\) since \(R_k\) are all different for all \(R_k \in C_{4v}\). In other terms, any eight-dimensional irrep of \(G\) is the regular representation of \(C_{4v}\). Thus, by the Burnside theorem, it breaks into \(A_1 \oplus A_2 \oplus B_1 \oplus B_2 \oplus E \oplus E\), with the two-dimensional irrep occurring twice; these are the symmetry labels of the local orbitals we are looking for. Now let \(k \in S_{hf}\). The only eigenvector of the matrix \(|R_k|\tilde{n}_{r=0}|R_k\rangle\) corresponding to the non-vanishing eigenvalue \(\lambda\) belongs to \(A_1\). Let \(R_k, i = 1, \ldots, 8\) denote respectively the identity \(1\), the counterclockwise and clockwise 90 degrees rotation \(C_4^+\), \(C_4^-\), the 180 degrees rotation \(C_2\), the reflection with respect to the \(y = 0\) and \(x = 0\) axis \(\sigma_x\), \(\sigma_y\) and the reflection with respect to the \(x = y\) and \(x = -y\) diagonals \(\sigma_{x}^\prime\), \(\sigma_{y}^\prime\). We can write down the eigenvectors of the above \(n_{r=0}\) matrix as \(|\psi_1^{(0)}\rangle = \sum_{i=1}^{8} O_{Ii} |R_k\rangle\), where \(k_x \geq k_y \geq 0\) and \(O\) is the \(8 \times 8\) orthogonal matrix

\[
O = \frac{1}{\sqrt{8}} \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 \\
1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\
-1 & -1 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix}.
\] (15)

Here, denoting by \(E'\) the second occurrence of the irrep \(E, I = 1, \ldots 8\) is the \(A_1, B_2, E_x, E_y, A_2, B_1, E'_x, E'_y\) irrep respectively. A translation by \(r\) yields the eigenstates \(|\psi_I^{(r)}\rangle\) of \(|R_k|\tilde{n}_r|R_k\rangle\) and of
the Dirac characters of the point symmetry group. After very long but elementary algebra one finds that the translation matrices \((T_I)_{IJ} = \langle \psi_J^{(0)} | \psi_I^{(e_i)} \rangle\) are

\[
T_x = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & \cos k_x & i \sin k_x & 0 \\
0 & 0 & 0 & 0 & \cos k_x & 0 & 0 & -i \sin k_x \\
0 & 0 & 0 & 0 & i \sin k_x & \cos k_x & 0 & 0 \\
0 & \cos k_x & 0 & i \sin k_x & 0 & 0 & 0 & 0 \\
\cos k_x & 0 & i \sin k_x & 0 & 0 & 0 & 0 & 0 \\
i \sin k_x & 0 & \cos k_x & 0 & 0 & 0 & 0 & 0 \\
0 & -i \sin k_x & 0 & -\cos k_x & 0 & 0 & 0 & 0
\end{pmatrix}
\]

(16)

and

\[
T_y = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & -\cos k_x & 0 & -i \sin k_x \\
0 & 0 & 0 & 0 & -\cos k_x & 0 & i \sin k_x & 0 \\
0 & 0 & 0 & 0 & i \sin k_x & -\cos k_x & 0 & 0 \\
0 & \cos k_x & 0 & i \sin k_x & 0 & 0 & 0 & 0 \\
-\cos k_x & 0 & i \sin k_x & 0 & 0 & 0 & 0 & 0 \\
i \sin k_x & -\cos k_x & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -i \sin k_x & 0 & 0 & 0 & 0 & 0 & \cos k_x
\end{pmatrix}
\]

(17)

where we have taken into account that at half filling \(k_y = \pi - k_x\). As for the two and four-dimensional irreps the translation matrices are in an antidiagonal block form; in particular they are such that the set containing the irreps \(A_1, B_2, E\) is mapped in the set containing the irreps \(A_2, B_1, E'\) and vice versa. This means that if we put 4 particles with spin \(\uparrow\) in the former 4 irreps and 4 particles with spin \(\downarrow\) in the latter 4 ones we obtain an 8-body state for which the translation by a lattice step is exactly equivalent to a spin-flip (antiferromagnetic property):

\[
|\psi_{A_1}^{(0)} \psi_{B_2}^{(0)} \psi_{E_x}^{(0)} \psi_{E_y}^{(0)} \rangle |\psi_{A_2}^{(0)} \psi_{B_1}^{(0)} \psi_{E_x'}^{(0)} \psi_{E_y'}^{(0)} \rangle - \sigma \longleftrightarrow |\psi_{A_2}^{(0)} \psi_{B_1}^{(0)} \psi_{E_x'}^{(0)} \psi_{E_y'}^{(0)} \rangle |\psi_{A_1}^{(0)} \psi_{B_2}^{(0)} \psi_{E_x}^{(0)} \psi_{E_y}^{(0)} \rangle - \sigma.
\]

(18)

Now recall that the occupation number vanishes for all the local states except the one of symmetry \(A_1\). Since in each site the \(A_1\) state of spin \(\sigma\) does not have the partner of the same symmetry with spin \(-\sigma\), the 8-body state of eq. (18) cannot have double occupancy on any site and therefore it is a \(W = 0\) state.

From now on we shall be engaged with the explicit construction of many-body \(W = 0\) states at half filling and it will be understood that we are using the local basis of the site \(r = 0\), so that \(|\psi^{(0)}\rangle \equiv |\psi\rangle\). We have observed above how the antiferromagnetic property of a many-particle determinant ensures that it is a \(W = 0\) state. In this way, we easily obtain a determinantal ground state of \(\hat{W}\) in \(\mathcal{H}\), i.e., at half filling, by creating holes in all the local orbitals of all the irreps, half with spin up and half with spin down. Let \(|\psi^{[m]}\rangle\) be the one-body eigenstate of \(n_r = 0\) belonging to the irrep \(I\) of \(C_{4v}\), in the space spanned by the basis functions of the \(m\)-th eight-dimensional irrep of \(G\). For even \(N/2\), the four-dimensional representation of \(G\) exists and the \(W = 0\) state wave function for the half filled case

\[
|\Phi_{AF}\rangle_\sigma \equiv \prod_{m=1}^{N_r} \psi_{A_1}^{[m]} \psi_{B_2}^{[m]} \psi_{E_x}^{[m]} \psi_{E_y}^{[m]} \psi_{A_1} \psi_{B_2} \psi_{A_1} \psi_{A_1} |\sigma\rangle \prod_{m=1}^{N_r} \psi_{A_2}^{[m]} \psi_{B_1}^{[m]} \psi_{E_x'}^{[m]} \psi_{E_y'}^{[m]} \psi_{E_x} \psi_{E_y} \psi_{B_1} |\sigma\rangle,
\]

(19)

with \(\sigma = \uparrow, \downarrow\) belongs to the first-order ground state multiplet (filled shells are understood, of course). For odd \(N/2\), on the other hand,

\[
|\Phi_{AF}\rangle_\sigma \equiv \prod_{m=1}^{N_r} \psi_{A_1}^{[m]} \psi_{B_2}^{[m]} \psi_{E_x}^{[m]} \psi_{E_y}^{[m]} |\sigma\rangle \prod_{m=1}^{N_r} \psi_{A_2}^{[m]} \psi_{B_1}^{[m]} \psi_{E_x'}^{[m]} \psi_{E_y'}^{[m]} |\sigma\rangle.
\]

(20)

We can see from eqs. (18) that \(|\Phi_{AF}\rangle_\sigma\) flips the spin and picks up a phase factor (see below) for each lattice step translation. Therefore, it manifestly shows an antiferromagnetic order (antiferromagnetic property). These results generalize Equation (11). In both cases, the \(-\sigma\) orbitals belong
to \( n_{t=0} = 0 \), and the antiferromagnetic property grants that the states are \( W = 0 \). Equivalently, we could have obtained a generalised version of (14) by building a basis of symmetry adapted eigenvectors of \( \sigma_i \) on the whole set \( S_{\text{plaq}} \), which can be done without handling large matrices.

A few further remarks about \( |\Phi_{AF}\rangle_\sigma \) are in order. 1) Introducing the projection operator \( P_S \) on the spin \( S \) subspace, one finds that \( P_S |\Phi_{AF}\rangle_\sigma \equiv |\Phi_{AF}\rangle_\sigma \neq 0 \), \( \forall S = 0, \ldots, N - 1 \). Then, \( \sigma (|\Phi_{AF}\rangle_W |\Phi_{AF}\rangle_\sigma = \sum_{S=1}^{N-1} \sigma (|\Phi_{AF}\rangle_W |\Phi_{AF}\rangle_\sigma = 0 \), and this implies that there is at least one \( W = 0 \) state of \( W \) in \( H \) for each \( S \). The ground state of \( H \) at weak coupling is the singlet \( |\Phi_{AF}\rangle_\sigma \). 2) The existence of this singlet \( W = 0 \) ground state is also a direct consequence of the Lieb theorem [10]. Indeed the maximum spin state \( |\Phi_{AF}^{N-1}\rangle_\sigma \) is trivially in the kernel of \( W \); since the ground state must be a singlet it should be an eigenvector of \( W \) with vanishing eigenvalue. 3) The above results and Lieb’s theorem imply that second and higher order effects split the ground state multiplet of \( H \) and the singlet is lowest. 4) The Lieb theorem makes no assumptions concerning the lattice structure; adding the ingredient of the \( G \) symmetry we are able to explicitly display the wave function at weak coupling.

In the next section we study the symmetries properties of the singlet component of \( |\Phi_{AF}\rangle_\sigma \).

### IV. SPIN PROJECTION AND SYMMETRIES OF \(|\Phi_{AF}\rangle\)

The \( W = 0 \) state \( |\Phi_{AF}\rangle_\sigma \) is a \( 2(N-1) \)-body determinantal state with \( S_z = 0 \) but is not an eigenstate of the total spin operator \( \hat{S}^z \). The various spin components are degenerate in first-order perturbation theory, but when higher-order effects are allowed the singlet component is lowest; if we wish to study the ground state of the Hubbard model we must project on the singlet. The spin projection operators \( P_S \) are well known and are reviewed in Appendix C for the sake of clarity. In order to find out the good quantum numbers of the ground state, the antisymmetric form

\[
|\Phi_{AF}\rangle \equiv \frac{|\Phi_{AF}\rangle_\sigma - |\Phi_{AF}\rangle_{-\sigma}}{\sqrt{2}}
\]

is more convenient to work with than the single determinant \( |\Phi_{AF}\rangle_\sigma \); using the explicit form of \( P_{S=0} \) one finds that the projection is the same.

#### A. symmetry under translations

Eqs. (10), (13), tell us that under a lattice step translation each of the determinantal states \( |\Phi_{AF}\rangle_\sigma \) of eqs. (15) undergoes a spin flip, which does not change the irreps of \( C_{4v} \) but modifies the order in which they appear in the many-body state. Since the fermion operators anticommute, the translated determinant is \(( -1)^{N-1} |\Phi_{AF}\rangle_{-\sigma} = - |\Phi_{AF}\rangle_{-\sigma} \); but in view of Equation (21), \( |\Phi_{AF}\rangle \rightarrow |\Phi_{AF}\rangle \) under a lattice step translation. Thus \( |\Phi_{AF}\rangle \) is an eigenstate of the total momentum with eigenvalue \( K_{\text{tot}} = (0, 0) \). Since the spin projection cannot change this quantum number, it holds for \( |\Phi_{AF}^{S=0}\rangle \) too.

#### B. reflections and rotations

Now we study how \( |\Phi_{AF}\rangle \) transforms under reflections and rotations with respect to the center of an arbitrary plaquette of the square lattice. We are not compelled to refer the operations to the center of a plaquette, rather than to a site, to characterize the symmetry properties of \( |\Phi_{AF}\rangle \); indeed the system is \( C_{4v} \) invariant in both cases. The only reason is to make contact with Ref. [11].

Since we represent sites by \( r = (i_x, i_y) \) with \( i_x, i_y = 0, \ldots, N - 1 \), we may choose the center at \( r_{\text{plaq}} = (1/2, 1/2) \). Let \( R_{\text{plaq}} \) denote the \( C_{4v} \) operations with respect to \( r_{\text{plaq}} \) and \( R \) the ones with respect to the origin \((0, 0)\). Then for every vector \( r \) of our lattice we have from elementary geometry

\[
R_{\text{plaq}} R_i r_{\text{plaq}} = R_i (r - r_{\text{plaq}}) + r_{\text{plaq}},
\]

(22)
This implies the transformation law for plane-wave states $|k\rangle$:

$$|k\rangle = \frac{1}{N} \sum_{r} e^{-ikr}|r\rangle \rightarrow |R_{\text{plaq}}^{I}k\rangle = \frac{1}{N} \sum_{r} e^{-ikr} |R_{\text{plaq}}^{I}r\rangle = e^{-i(kR_{\text{plaq}}-R_{\text{plaq}}^{-1}kR_{\text{plaq}})}|R_{I}k\rangle,$$  \hspace{1cm} (23)

where the last equality can be obtained with a change of variables. By means of eq. (23) it is possible to know how each irrep of the space group $G$ transforms.

Two-dimensional irrep: Let us first consider the two-dimensional irrep whose basis vectors are $|\psi_{A1}'\rangle = \frac{1}{\sqrt{N}}(|kA\rangle + |kB\rangle)$ and $|\psi_{B1}'\rangle = \frac{1}{\sqrt{N}}(|kA\rangle - |kB\rangle)$. Under $R_{\text{plaq}}^{I}$ we have

$$|\psi_{A1}'\rangle \rightarrow |R_{\text{plaq}}^{I}\psi_{A1}'\rangle = \frac{1}{\sqrt{2}}(|R_{\text{plaq}}^{I}kA\rangle + |R_{\text{plaq}}^{I}kB\rangle),$$

$$|\psi_{B1}'\rangle \rightarrow |R_{\text{plaq}}^{I}\psi_{B1}'\rangle = \frac{1}{\sqrt{2}}(|R_{\text{plaq}}^{I}kA\rangle - |R_{\text{plaq}}^{I}kB\rangle).$$  \hspace{1cm} (24)

The transformed local states $|R_{\text{plaq}}^{I}\psi_{f}'\rangle$, with $I = A_{1}, B_{1}$, can be expressed in terms of the original ones $|\psi_{f}'\rangle$:

$$|R_{\text{plaq}}^{I}\psi_{f}'\rangle = \sum_{J=A_{1}, B_{1}}|\psi_{J}'\rangle \langle \psi_{J}'|R_{\text{plaq}}^{I}\psi_{f}'\rangle$$  \hspace{1cm} (25)

Using eqs. (23) and computing the overlaps $\langle \psi_{J}'|R_{\text{plaq}}^{I}\psi_{f}'\rangle$ of eq. (25), we have studied how the $W = 0$ pair state in eq. (6) transforms under a 90 degrees rotation $C_{4}^{(+)}$ and a reflection with respect to the $y = 0$ and $x = y$ axis $\sigma_{x}$ and $\sigma_{+}$ respectively. After some algebra it is possible to show that

$$|\psi_{A1}'\rangle_{\sigma}|\psi_{B1}'\rangle_{-\sigma} \leftrightarrow -|\psi_{B1}'\rangle_{\sigma}|\psi_{A1}'\rangle_{-\sigma} \hspace{1cm} C_{4}^{(+)}$$

$$|\psi_{A1}'\rangle_{\sigma}|\psi_{B1}'\rangle_{-\sigma} \leftrightarrow |\psi_{B1}'\rangle_{\sigma}|\psi_{A1}'\rangle_{-\sigma} \hspace{1cm} \sigma_{x}$$

$$|\psi_{A1}'\rangle_{\sigma}|\psi_{B1}'\rangle_{-\sigma} \leftrightarrow -|\psi_{A1}'\rangle_{\sigma}|\psi_{B1}'\rangle_{-\sigma} \hspace{1cm} \sigma_{+}.$$  \hspace{1cm} (26)

where $\leftrightarrow$ means that the left hand side transforms in the right hand side and conversely under the operation specified on the right.

For a $2 \times 2$ square lattice the two-dimensional irrep is the only one in $S_{hf}$ and $|\Phi_{AF}\rangle$ is explicitly given by

$$|\Phi_{AF}\rangle = |\psi_{A1}'\rangle_{\sigma}|\psi_{B1}'\rangle_{-\sigma} + |\psi_{B1}'\rangle_{\sigma}|\psi_{A1}'\rangle_{-\sigma}. $$  \hspace{1cm} (27)

By means of eqs. (24) it is not hard to see that $|\Phi_{AF}\rangle$ transforms as a d wave of $x^{2} - y^{2}$ symmetry. This symmetry property cannot change after the spin projection of $|\Phi_{AF}\rangle$ on the $S = 0$ subspace and we conclude that $|\Phi_{AF}^{S=0}\rangle$ transforms as a d wave too. Finally we observe the the $2 \times 2$ case is special because $|\Phi_{AF}\rangle$ is already a singlet and then must coincide with $|\Phi_{AF}^{S=0}\rangle$. This will be no more true if $N \geq 4$.

Four-dimensional irrep: Similarly we can study the behaviour of the four-body $W = 0$ state of eq. (14) under the three operations in eq. (24). One finds:

$$|\psi_{A1}'\psi_{B1}'\psi_{E_{x}}'\psi_{E_{y}}'\rangle_{\sigma} \leftrightarrow -|\psi_{E_{x}}'\psi_{E_{y}}'\psi_{A1}'\psi_{B1}'\rangle_{-\sigma} \hspace{1cm} C_{4}^{(+)}$$

$$|\psi_{A1}'\psi_{B1}'\psi_{E_{x}}'\psi_{E_{y}}'\rangle_{\sigma} \leftrightarrow |\psi_{E_{x}}'\psi_{E_{y}}'\psi_{A1}'\psi_{B1}'\rangle_{-\sigma} \hspace{1cm} \sigma_{x}$$

$$|\psi_{A1}'\psi_{B1}'\psi_{E_{x}}'\psi_{E_{y}}'\rangle_{\sigma} \leftrightarrow -|\psi_{A1}'\psi_{B1}'\psi_{E_{x}}'\psi_{E_{y}}'\rangle_{-\sigma} \hspace{1cm} \sigma_{+}.$$  \hspace{1cm} (28)

A remarkable feature follows from the above transformation properties. In the $N = 4$ case $S_{hf}$ contains the irrep of dimension 2 and the one of dimension 4 so that $|\Phi_{AF}\rangle$ is

$$|\Phi_{AF}\rangle = |\psi_{A1}'\psi_{B1}'\psi_{E_{x}}'\psi_{E_{y}}'\rangle_{\sigma} |\psi_{E_{x}}'\psi_{E_{y}}'\psi_{B1}'\rangle_{-\sigma} + |\psi_{E_{x}}'\psi_{E_{y}}'\psi_{B1}'\rangle_{\sigma} |\psi_{A1}'\psi_{B1}'\psi_{E_{x}}'\psi_{E_{y}}'\rangle_{-\sigma}. $$  \hspace{1cm} (29)
Using eqs. (23) (28) it can be shown that \( |\Phi_{AF} \rangle \) transforms as an \( s \) wave of \( x^2 + y^2 \) symmetry for \( N = 4 \). Therefore the symmetry of \( |\Phi_{AF} \rangle \) depends on \( N \) and the next step will be to determine how this happens. To this end we need the transformation properties of an arbitrary 8-dimensional irrep of \( G \) contained in \( S_{hf} \).

Eight-dimensional irrep:

After very long but simple algebra we have found that the eight-body state of eq. (28) transforms as

\[
\begin{align*}
|\psi_{A_1}\psi_{B_2}\psi_{E_2}\psi_{E_2}^{\sigma}\rangle |\psi_{A_2}\psi_{B_1}\psi_{E_1}\psi_{E_1}^{\sigma}\rangle & \leftrightarrow |\psi_{A_1}\psi_{B_1}\psi_{E_1}\psi_{E_1}^{\sigma}\rangle |\psi_{A_2}\psi_{B_2}\psi_{E_2}\psi_{E_2}^{\sigma}\rangle - \sigma \ C_4^{(s)} \\
|\psi_{A_1}\psi_{B_2}\psi_{E_2}\psi_{E_2}^{\sigma}\rangle |\psi_{A_2}\psi_{B_1}\psi_{E_1}\psi_{E_1}^{\sigma}\rangle & \leftrightarrow |\psi_{A_1}\psi_{B_1}\psi_{E_1}\psi_{E_1}^{\sigma}\rangle |\psi_{A_2}\psi_{B_2}\psi_{E_2}\psi_{E_2}^{\sigma}\rangle - \sigma_x \\
|\psi_{A_1}\psi_{B_2}\psi_{E_2}\psi_{E_2}^{\sigma}\rangle |\psi_{A_2}\psi_{B_1}\psi_{E_1}\psi_{E_1}^{\sigma}\rangle & \leftrightarrow |\psi_{A_1}\psi_{B_1}\psi_{E_1}\psi_{E_1}^{\sigma}\rangle |\psi_{A_2}\psi_{B_2}\psi_{E_2}\psi_{E_2}^{\sigma}\rangle - \sigma'_x.
\end{align*}
\]

(30)

For \( k_x \to \pi/2 \) the 8-dimensional irrep is equivalent to two 4-dimensional ones and the eqs. (30) are the “square” of the eqs. (28). Analogously for \( k_x \to \pi \) we obtain four times the 2-dimensional irrep and eqs. (30) are the “fourth power” of eqs. (28).

From (11) we deduce that whatever is the number of 8-dimensional irreps, the symmetry of \( |\Phi_{AF} \rangle \) depends only by the presence or absence of the 4-dimensional one. More exactly if \( N/2 \) is even \( |\Phi_{AF} \rangle \) belongs to the one-dimensional irrep \( A_1 \) and if \( N/2 \) is odd to the one-dimensional irrep \( B_1 \).

As noted at the beginning of this section, the spin projection on the singlet subspace does not alter the above quantum numbers. Therefore we conclude that the \( W = 0 \) singlet state \( |\Phi^{S_{AF} = 0} \rangle \) has total momentum \( K_{tot} = (0, 0) \) and transforms as a \( d \) wave of \( x^2 + y^2 \) symmetry if \( N/2 \) is odd and as an \( s \) wave of \( x^2 + y^2 \) symmetry if \( N/2 \) is even. The same quantum numbers were obtained in Ref. [11] for the ground state of the Hubbard model in the opposite, strong coupling regime. This coincidence is a further consequence of Lieb’s theorem. Since the ground state at half filling must be unique, no level crossing is allowed for finite \( U \), and the symmetry of the ground state is the same at weak and strong coupling.

V. ACKNOWLEDGEMENTS

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APPENDIX A: CONTRIBUTIONS TO THE \( \hat{W} \) MATRIX FROM FILLED SHELLS

The \( N^2 \)–body determinantal wave functions with \( S_z = 0 \) that one can build using the orbitals with \( \epsilon(k) < 0 \) and half of those with \( \epsilon(k) = 0 \) are a set of \( \left( \begin{array}{c} 2N - 2 \\ N - 1 \end{array} \right) \) elements. Each represents one of the degenerate unperturbed \( (U = 0) \) ground state configurations at half filling. First-order perturbation theory requires the diagonalization of the \( W \) matrix over such a basis.

The diagonal elements of the \( W \) matrix are just expectation values over determinants \( |k_\alpha \uparrow k_\beta \downarrow \ldots \rangle \). Such an expectation value is a sum over all the possible pairs of the bielectronic elements of \( W \) like

\[
W(\alpha\beta,\alpha\beta) = \sum_r U(k_\alpha|n_r|k_\alpha) \langle k_\beta|n_r|k_\beta \rangle
\]

\[
= \sum_r \frac{U}{N^2} \frac{1}{N^2} e^{i(k_\alpha - k_\beta) r} = \frac{U}{N^4} N^2 = \frac{U}{N^2}.
\]

(A1)

the result is independent of \( k_\alpha \) and \( k_\beta \). Since in any determinant of the set \( N^2/2 \) plane wave states are occupied for each spin, there are \( N^4/4 \) pairs, and the diagonal elements are all equal to \( UN^2/4 \). Thus, the diagonal elements shift all the eigenvalues by this fixed amount.

The off-diagonal elements of the \( W \) matrix between determinants that differ by three or more spin-orbitals vanish because \( \hat{W} \) is a two-body operator. The off-diagonal elements between determinants that differ by one spin-orbital are sum of contributions like \( W(\alpha\beta,\gamma\beta) = \sum_r U(k_\alpha|n_r|k_\gamma) \langle k_\beta|n_r|k_\beta \rangle \) that vanish because of the orthogonality of the plane-wave orbitals. One is left with the off-diagonal
elements between determinants that differ by two spin-orbitals, which coincide with the corresponding bielectronic elements \( W(\alpha\beta, \gamma\delta) = \sum_r U(k_\alpha|n_r|k_\gamma)(k_\beta|n_r|k_\delta) \). This is just the matrix of \( W \) over the truncated Hilbert space \( \mathcal{H} \) spanned by the states of the holes in the half filled shell, ignoring the filled ones. We stress that there are \( N - 1 \) holes of each spin in \( S_{hf} \), thus \( \mathcal{H} \) is much smaller than the full Hilbert space of the Hubbard Hamiltonian; however, since the number of holes grows linearly with \( N \), the problem is still far from trivial.

**APPENDIX B: EIGENVALUES OF THE NUMBER OPERATOR**

Here we prove Equation (4). Expanding the determinant according to its definition in terms of the totally antisymmetric tensor \( \epsilon \),

\[
det | (n_r)_{ij} - \lambda \delta_{ij} | = \sum_{i_1 \ldots i_{|\mathcal{S}|}} \epsilon_{i_1 \ldots i_{|\mathcal{S}|}} \left( \frac{1}{N^2} e^{i(k_1 - k_{i_1}) r} - \lambda \delta_{i_1, i} \right) \ldots \left( \frac{1}{N^2} e^{i(k_{|\mathcal{S}|} - k_{i_{|\mathcal{S}|}}) r} - \lambda \delta_{|\mathcal{S}|, i_{|\mathcal{S}|}} \right) \quad (B1)
\]

we see that the term of maximum order in \( \lambda \) is \((-\lambda)^{|\mathcal{S}|}\); it arises from the fundamental permutation \((i_1, i_2, \ldots) \equiv (1, 2, \ldots)\). The \((|\mathcal{S}| - 1)\)-th order term in \( \lambda \) is the sum of \(|\mathcal{S}|\) identical contributions also arising from the fundamental permutation. Therefore, it is

\[
\frac{|\mathcal{S}|}{N^2} (-\lambda)^{|\mathcal{S}| - 1}. \quad (B2)
\]

It is not difficult to see that all the other orders in \( \lambda \) yield nothing. At order zero one finds

\[
\frac{1}{N^2 |\mathcal{S}|} \sum_{i_1 \ldots i_{|\mathcal{S}|}} \epsilon_{i_1 \ldots i_{|\mathcal{S}|}} e^{i(k_1 + \ldots + k_{|\mathcal{S}|} - k_{i_1} - \ldots - k_{i_{|\mathcal{S}|}}) r}. \quad (B3)
\]

Since the exponential is totally symmetric in the permutation of \( i_1 \ldots i_{|\mathcal{S}|} \) while \( \epsilon \) is totally antisymmetric the sum vanishes.

Now we analyze the first order term in \( \lambda \). One of its contributions is obtained by picking \(-\lambda\) in the first factor of eq.(B1), i.e. by setting \( i_1 = 1 \). This contribution can be written as

\[
\frac{1}{N^2 (|\mathcal{S}| - 1)} \sum_{i_2 \ldots i_{|\mathcal{S}|}} \epsilon_{i_2 \ldots i_{|\mathcal{S}|}} e^{i(k_2 + \ldots + k_{|\mathcal{S}|} - k_{i_2} - \ldots - k_{i_{|\mathcal{S}|}}) r}. \quad (B4)
\]

Again, the exponential is symmetric \( i_2 \ldots i_{|\mathcal{S}|} \) and the sum in eq.(B4) vanishes. Clearly, this argument applies to all the contributions to first order and to all orders less than \(|\mathcal{S}| - 1\).

So, we are left with the only two nonvanishing terms,

\[
det | n_r - \lambda | = (-\lambda)^{|\mathcal{S}| - 1} \left( \frac{|\mathcal{S}|}{N^2} - \lambda \right) \quad (B5)
\]

that is, eq.(4).

**APPENDIX C: SPIN PROJECTION OPERATORS \( P_S \)**

Let us consider a determinantal state with \( 2n \) spin-orbitals, half of spin up and half of spin down, like

\[
|\Psi\rangle_\sigma \equiv |\psi_1 \ldots \psi_n\rangle_\sigma |\psi_{n+1} \ldots \psi_{2n}\rangle_{-\sigma} \quad (C1)
\]

with \( \langle \psi_i | \psi_j \rangle = \delta_{ij} \). Due to the anticommuting property of the fermionic operators, \( |\psi\rangle \) is separately antisymmetric in the indices \( 1, \ldots, n \) and \( n + 1, \ldots, 2n \). \( |\Psi\rangle_\sigma \) is no eigenstate of \( S^2 \) and \( \forall S = 0, \ldots, n, \ P_S |\Psi\rangle_\sigma \neq 0 \). To build \( P_S \), we take advantage of the fact that different \( S \) correspond to different irreps.
of the Permutation Group of the spins. To this end, let us draw the following table, or Young Tableau

\[
\begin{array}{cccccccc}
1 & 2 & \ldots & i_{n-S} & j_{n-S+1} & \ldots & i_{n+S} \\
1 & 2 & \ldots & j_{n-S} & & & \\
\end{array}
\]

(C2)

where the values of the indices \(i_k\) and \(j_k\) must be a permutation of \(1, \ldots, 2n\) with the constraints 1) \(i_k < j_k\ \forall k = 1, \ldots, n - S\) and 2) \(i_k < i_{k+1}, j_k < j_{k+1}\). Now we define \(C_{i,j}\) as the operator that exchanges the spins of the \(|\psi_i\rangle\) and \(|\psi_j\rangle\) states; we associate to the above table the operator

\[
\prod_{a=1}^{n+S-1} (1 + \sum_{\alpha=1}^{n+S-a} C_{i_{a,i_{n+S-a+1}}}) \prod_{b=1}^{n-S-1} (1 + \sum_{\beta=1}^{n-S-b} C_{j_{\beta,j_{n-S-b+1}}}) \prod_{l=1}^{n-S} (1 - C_{i_l,j_l}).
\]

(C3)

This operator antisymmetrizes the indices on the same column and then symmetrizes those on the same row. Then \(P_S\) is proportional, up to a normalization factor, to the sum of the operators associated to all tables (C2) that comply with the constraints 1) and 2).

Example: \(n = 2 \Rightarrow |\Psi\rangle_\sigma = |\psi_1 \uparrow \psi_2 \uparrow \psi_3 \downarrow \psi_4 \downarrow \rangle \equiv |\psi_1 \psi_2 \rangle \uparrow |\psi_3 \psi_4 \rangle \downarrow\). In this case the three projection operators are

\[
P_{S=2} \propto \begin{array}{ccc}
1 & 2 & 3 \\
4 & & \\
\end{array}
\]

\[
P_{S=1} \propto \begin{array}{ccc}
1 & 2 & 3 \\
4 & & \\
3 & & \\
2 & & \\
\end{array} + \begin{array}{ccc}
1 & 2 & 4 \\
3 & & \\
2 & & \\
\end{array} + \begin{array}{ccc}
1 & 3 & 4 \\
2 & & \\
\end{array}
\]

(C4)

\[
P_{S=0} \propto \begin{array}{ccc}
1 & 2 & 3 \\
4 & & \\
3 & & \\
2 & & \\
\end{array} + \begin{array}{ccc}
1 & 2 & 4 \\
3 & & \\
2 & & \\
\end{array} + \begin{array}{ccc}
1 & 3 & 4 \\
2 & & \\
\end{array}
\]

If a table has two indices corresponding to states with equal spin in the same column, the action of the associated operator on \(|\Psi\rangle_\sigma\) will yield zero. This means that in the above example we can omit the third table of \(P_{S=1}\) and the second one of \(P_{S=0}\). We have special interest in \(P_{S=0}\), which projects on the totally antisymmetric irrep. For all \(n\), it always consists of only one table

\[
P_{S=0} = \begin{array}{ccc}
1 & 2 & \ldots & n \\
1 + n & 2 + n & \ldots & 2n \\
\end{array}
\]

(C5)

Using the explicit form of \(P_{S=0}\) one finds that the singlet projection contains \(|\Psi\rangle_\sigma\) and \(|\Psi\rangle_{-\sigma}\) in a combination, which is symmetric for even \(n\) and antisymmetric if \(n\) is odd.

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$C_{4v}$ is the symmetry group of a square. It is a finite group of order 8 and it contains 4 one dimensional irreps, $A_1$, $A_2$, $B_1$, $B_2$, and 1 two-dimensional one called $E$. The table of characters is

| $C_{4v}$ | 1 | $C_2$ | $C_4^{(+)}$, $C_4^{(-)}$ | $\sigma_x$, $\sigma_y$, $\sigma'_x$, $\sigma'_y$ |
|----------|---|-------|--------------------------|-----------------------------------------------|
| $A_1$    | 1 | 1     | 1                        | 1, 1                                         |
| $A_2$    | 1 | 1     | 1                        | -1, -1                                       |
| $B_1$    | 1 | 1     | -1                       | 1, -1                                        |
| $B_2$    | 1 | 1     | -1                       | -1, 1                                        |
| $E$      | 2 | -2    | 0                        | 0, 0                                         |

[14] Morton Hamermesh, *Group Theory and its application to Physical Problems*, Addison-Wesley (reading, 1962).

[15] Equivalently, we shall find the exact $2N - 2$-body ground state of the effective Hamiltonian

$$H_{\text{eff}} = \frac{U}{N^4} \sum_{k_1,k_2,k_3,k_4 \in \mathcal{S}_{hf}} \delta(k_1 + k_2 - k_3 - k_4)c_{k_1}^{\dagger}c_{k_2}^{\dagger}c_{k_3}c_{k_4}$$

(C6)

where $\delta(G) = 1$ if $G$ is a reciprocal lattice vector and zero otherwise.

[16] Michele Cini, Adalberto Balzarotti, Raffaella Brunetti, Maria Gimelli and Gianluca Stefanucci, International J. of Modern Physics, in press.

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[19] We recall that the $W = 0$ state $|\Phi_{AF}\rangle_\sigma$ is of this form, with $n = N - 1$.

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