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Antiferromagnetism of the two-dimensional Hubbard model at half-filling: the analytic ground state for weak coupling

Michele Cini and Gianluca Stefanucci

Istituto Nazionale di Fisica della Materia, Dipartimento di Fisica,
Università di Roma Tor Vergata, Via della Ricerca Scientifica, 1-00133 Roma, Italy

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Abstract

We introduce a *local* formalism to deal with the Hubbard model on an $N \times N$ 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 $\mathcal{S}_{hf}$, we build a set of $\binom{2N-2}{N-1}$ degenerate unperturbed ground states with $S_z = 0$ which are then resolved by the Hubbard interaction $\hat{W} = U \sum_r \hat{n}_{r\uparrow}\hat{n}_{r\downarrow}$. We study the many-body eigenstates in $\mathcal{S}_{hf}$ of the kinetic energy with vanishing eigenvalue of the Hubbard repulsion ($W = 0$ states). In the $S_z = 0$ sector, this is an 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 of Lieb. The wave function demonstrates an antiferromagnetic order, a lattice step translation being equivalent to a spin flip. We show that the total momentum vanishes, while the point symmetry is s or d for even or odd $N/2$, respectively.

1. Introduction

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 idealized—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 (whose limitations are discussed in reference [3]), which is based on a conservation approximation and, independently, renormalization group techniques [4,5] show that near the antiferromagnetic phase at half-filling, there exists a superconducting phase too, with a momentum-dependent gap, of d-wave symmetry. An indication of a possible instability of the Fermi liquid towards pairing near half-filling also comes from cluster diagonalizations [6–8]. Therefore, exact results on the half-filled Hubbard model may be relevant to antiferromagnetism and to the mechanism of the superconducting instability as well.

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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 [9]. A popular approach takes care of the strong repulsion between two opposite spin fermions by means of a Gutzwiller [10] 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, and even in the ground state, although its probability decreases steadily with increasing U. There is strong evidence that the results obtained for weak coupling by perturbation theory compare well with available numerical results even for intermediate coupling [11] (a more extensive study concerning the applicability of Goldstone perturbation theory to the Hubbard model is discussed in reference [12]). For weak coupling it makes sense to speak of particles in filled shells, which behave much like 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 by 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 [13]: the ground state for a bipartite lattice is unique and has spin $\frac{1}{2}||\mathcal{S}_1| - |\mathcal{S}_2||$ where $|\mathcal{S}_1|$ ($|\mathcal{S}_2|$) is the number of sites in the $\mathcal{S}_1$ ($\mathcal{S}_2$) sublattice; here and in the following, $|\mathcal{S}|$ will be the number of elements in the set $\mathcal{S}$. It is worth observing that the theorem makes no assumptions about the symmetry of the lattice. For an $N \times N$ square lattice, with N even, the ground state is a singlet and in reference [14] 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 for weak coupling. In section 2 we state more precisely the problem that we want to solve and we define some notation. In section 3 we show how for each site we can build a *local* one-body basis set, which is well suited as a basis in which to expand the antiferromagnetic many-body wave function. Finally in section 4 we explore the symmetry properties of the ground state, and deduce the same quantum numbers as were predicted by references [13, 14] for strong coupling.

The present approach is new (to the best of our knowledge) and lends itself to several further applications, although, admittedly, it is limited to finite N (that is, N may be arbitrarily large but we cannot take the $N \to \infty$ limit at the start). We can also obtain exact results for other fillings as well, but this will be shown elsewhere [15].

2. The Hubbard model at half-filling and for weak coupling

Let us consider the Hubbard model with Hamiltonian

$$H = H_0 + \hat{W} = t \sum_{\sigma} \sum_{\langle r,r' \rangle} c^{\dagger}_{r\sigma} c_{r'\sigma} + \sum_{r} U \hat{n}_{r\uparrow} \hat{n}_{r\downarrow} \qquad U > 0 \tag{1}$$

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' are 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-neighbour sites and $\hat{n}_{r\sigma}$ is the number operator on the site r of spin σ. The point symmetry is C_{4v}, the group

of a square[1]; also, H is invariant under the commutative group of translations $\mathbf{T}$ and hence the space group [16] $\mathbf{G} = \mathbf{T} \otimes \mathrm{C_{4v}}$; $\otimes$ 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

$$c_{k\sigma} = \frac{1}{N}\sum_r \mathrm{e}^{\mathrm{i}kr} c_{r\sigma}$$

we have

$$H_0 = \sum_k \epsilon(k) c^\dagger_{k\sigma} c_{k\sigma}$$

with $\epsilon(k) = 2t[\cos k_x + \cos k_y]$. Then the one-body plane-wave state $c^\dagger_{k\sigma}|0\rangle \equiv |k\sigma\rangle$ is an eigenstate of H_0.

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

$$\begin{aligned} \hat{S}_z &= \frac{1}{2}\sum_r (\hat{n}_{r\uparrow} - \hat{n}_{r\downarrow}) \\ \hat{S}^+ &= \sum_r c^\dagger_{r\uparrow} c_{r\downarrow} \\ \hat{S}^- &= (\hat{S}^+)^\dagger \end{aligned} \tag{2}$$

at half-filling every ground state of H_0 is represented in the $S_z = 0$ subspace. Thus, H_0 has $\binom{2N-2}{N-1}$ 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* $\mathcal{S}_{hf}$. Equivalently, one solves a $(2N-2)$-particle problem in the truncated Hilbert space $\mathcal{H}$ and then, taking into account that the contribution of the particles in the shells that are completely filled factors out, one 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.

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

$\mathrm{C_{4v}}$	**1**	$\mathrm{C_2}$	$\mathrm{C_4^{(+)}}, \mathrm{C_4^{(-)}}$	$\sigma_x,\ \sigma_y$	$\sigma'_+,\ \sigma'_-$
$\mathrm{A_1}$	1	1	1	1	1
$\mathrm{A_2}$	1	1	1	−1	−1
$\mathrm{B_1}$	1	1	−1	1	−1
$\mathrm{B_2}$	1	1	−1	−1	1
E	2	−2	0	0	0

The operator $\sum_r \hat{n}_{r\uparrow}\hat{n}_{r\downarrow}$ has eigenvalues 0, 1, 2, ... and so the lowest eigenvalue of $\hat{W}$ is zero (in other words, $\hat{W}$ 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 $\mathcal{S}_{hf}$ (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[2].

3. *Local* formalism for the ground-state wave function

In this 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 4×4 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.

3.1. The basis set: definition

Since $\hat{W}$ depends on the occupation number operators $\hat{n}_r$, it is intuitively obvious that its properties in $\mathcal{H}$ are best discussed by using 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 high **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 (*irrep*); thus we write the one-body basis states as $\{|\varphi_\alpha^{(r)}\rangle\}$ where α comprises the $\hat{n}_r$-eigenvalue and a C_{4v} irrep label. However, different sites yield different sets; the eigenvectors $|\varphi_\alpha^{(0)}\rangle$ of $n_{r=0}$ and those ($|\varphi_\alpha^{(r)}\rangle$) 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

$$|\varphi_\alpha^{(\hat{e}_l)}\rangle = \sum_{\beta=1}^{2N-2} |\varphi_\beta^{(0)}\rangle\langle\varphi_\beta^{(0)}|\varphi_\alpha^{(\hat{e}_l)}\rangle \equiv \sum_{\beta=1}^{2N-2} |\varphi_\beta^{(0)}\rangle T_{l_{\beta\alpha}} \qquad l = x, y. \tag{4}$$

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.

3.2. The technique for building the basis set

To accomplish this, 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 using the following:

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

$$H_{eff} = \frac{U}{N^4} \sum_{k_1,k_2,k_3,k_4 \in \mathcal{S}_{hf}} \delta(k_1 + k_2 - k_3 - k_4) c_{k_1\uparrow}^\dagger c_{k_2\downarrow}^\dagger c_{k_3\downarrow} c_{k_4\uparrow} \tag{3}$$

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

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

Note that $|\mathcal{S}| \leqslant N^2$; if $|\mathcal{S}| = N^2$ 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)

$$\det|(n_r)_{ij} - \lambda\delta_{ij}| = (-\lambda)^{|\mathcal{S}|-1}\left(\frac{|\mathcal{S}|}{N^2} - \lambda\right) \qquad \forall r. \tag{5}$$

It is easy to verify that for $r = 0$ the eigenvector with non-zero eigenvalue is just the totally symmetric superposition of all the $\{|k_i\rangle\} \in \mathcal{S}$.

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 $k_x \geqslant k_y \geqslant 0$. 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 $k_x \geqslant k_y \geqslant 0$, and hence $k_x + k_y = \pi$, the set of vectors $R_i k \in \mathcal{S}_{hf}$, where $R_i \in C_{4v}$, 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 wave vectors $k = (\pm\pi/2, \pm\pi/2)$ which mix among themselves and yield a four-dimensional irrep. In general, when k is not in a special symmetry direction, the vectors $R_i k$ are all different, so all of 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 + 4 times that of four-dimensional ones + 2 for the only two-dimensional irrep must yield $|\mathcal{S}_{hf}| = 2N - 2$, one finds that $\mathcal{S}_{hf}$ contains $N_e = \frac{1}{2}(N/2 - 2)$ irreps of dimension 8 if $N/2$ is even and $N_o = \frac{1}{2}(N/2 - 1)$ irreps of dimension 8 if $N/2$ is odd.

We note incidentally that **G** cannot explain the degeneracy $2N - 2$ of $\mathcal{S}_{hf}$, 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 reference [17].

In this way, $\mathcal{S}_{hf}$ is seen to be the union of disjoint bases of different irreps of the space group. This break-up of $\mathcal{S}_{hf}$ 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.

3.3. Example: the basis set and ground state for the 4×4 *square lattice*

As already noted, $k_A = (\pi, 0)$ and $k_B = (0, \pi)$ belong to $\mathcal{S}_{hf}$ and are the basis of a two-dimensional irrep of **G**. The 2×2 matrix $(n_{r=0})_{ij} = \langle k_i|\hat{n}_{r=0}|k_j\rangle$, with $i, j = A, B$, has the eigenvector

$$|\psi^{\prime\prime(0)}_{A_1}\rangle = \frac{1}{\sqrt{2}}(|k_A\rangle + |k_B\rangle)$$

with eigenvalue $\lambda_1 = 1/8$, in agreement with the above theorem. The second eigenvector, with vanishing eigenvalue, is

$$|\psi^{\prime\prime(0)}_{B_1}\rangle = \frac{1}{\sqrt{2}}(|k_A\rangle - |k_B\rangle).$$

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: $|k\rangle \to \mathrm{e}^{\mathrm{i}kr}|k\rangle$. Thus, the eigenstates of n_r are

$$|\psi''^{(r)}_{\mathrm{A}_1}\rangle = \frac{1}{\sqrt{2}}(\mathrm{e}^{\mathrm{i}k_{\mathrm{A}}r}|k_{\mathrm{A}}\rangle + \mathrm{e}^{\mathrm{i}k_{\mathrm{B}}r}|k_{\mathrm{B}}\rangle)$$

with $\lambda_1 = 1/8$ and

$$|\psi''^{(r)}_{\mathrm{B}_1}\rangle = \frac{1}{\sqrt{2}}(\mathrm{e}^{\mathrm{i}k_{\mathrm{A}}r}|k_{\mathrm{A}}\rangle - \mathrm{e}^{\mathrm{i}k_{\mathrm{B}}r}|k_{\mathrm{B}}\rangle)$$

with $\lambda_2 = 0$. The primitive translations (4) are performed as follows:

$$|\psi''^{(\hat{e}_l)}_I\rangle = \sum_{J=\mathrm{A}_1,\mathrm{B}_1} |\psi''^{(0)}_J\rangle\langle\psi''^{(0)}_J|\psi''^{(\hat{e}_l)}_I\rangle \equiv \sum_{J=\mathrm{A}_1,\mathrm{B}_1} |\psi''^{(0)}_J\rangle(T_l)_{JI} \qquad l = x, y \tag{6}$$

with $I = \mathrm{A}_1, \mathrm{B}_1$. Using equation (6) one finds the antidiagonal translation matrices T_l:

$$T_x = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \qquad T_y = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{7}$$

So, the orbital of A_1 symmetry at $r = 0$ has B_1 symmetry around the nearest-neighbour sites, and conversely. In particular, $|\psi''^{(0)}_{\mathrm{A}_1}\rangle$ has vanishing amplitude on a sublattice and $|\psi''^{(0)}_{\mathrm{B}_1}\rangle$ on the other. The two-body state $|\psi''^{(0)}_{\mathrm{A}_1}\rangle_\sigma|\psi''^{(0)}_{\mathrm{B}_1}\rangle_{-\sigma}$ has occupation for spin σ 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:

$$|\psi''^{(0)}_{\mathrm{A}_1}\rangle_\sigma|\psi''^{(0)}_{\mathrm{B}_1}\rangle_{-\sigma} \longleftrightarrow |\psi''^{(0)}_{\mathrm{B}_1}\rangle_\sigma|\psi''^{(0)}_{\mathrm{A}_1}\rangle_{-\sigma} = -|\psi''^{(0)}_{\mathrm{A}_1}\rangle_{-\sigma}|\psi''^{(0)}_{\mathrm{B}_1}\rangle_\sigma. \tag{8}$$

Therefore it has double occupation nowhere and is a $W = 0$ state (more precisely, a $W = 0$ pair [18, 19]).

For $N = 4$, $\mathcal{S}_{hf}$ 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 four-dimensional irrep of $\mathbf{G}$. This irrep breaks into $\mathrm{A}_1 \oplus \mathrm{B}_2 \oplus \mathrm{E}$ in $\mathrm{C}_{4\mathrm{v}}$, and such are the symmetry labels of the eigenvectors of $\hat{n}_{r=0}$. We easily obtain them using the projection operators of $\mathrm{C}_{4\mathrm{v}}$. Letting $I = 1, 2, 3, 4$ for the irreps $\mathrm{A}_1, \mathrm{B}_2, \mathrm{E}_x, \mathrm{E}_y$ respectively, we can write down all the eigenvectors of $\langle k_i|\hat{n}_{r=0}|k_j\rangle$, with $i, j = 1, \ldots, 4$, as

$$|\psi'^{(0)}_I\rangle = \sum_{i=1}^{4} O'_{Ii}|k_i\rangle$$

where O' is the following 4×4 orthogonal matrix:

$$O' = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & -1 & 1 & 1 \end{bmatrix}. \tag{9}$$

The state with non-vanishing eigenvalue is again of A_1 symmetry. Translating by r we readily get the eigenstates $|\psi'^{(r)}_I\rangle$ of n_r and of the Dirac characters; in this way, we calculate the translation matrices $(T_l)_{JI} = \langle\psi'^{(0)}_J|\psi'^{(\hat{e}_l)}_I\rangle$, which are block-antidiagonal:

$$T_x = \begin{bmatrix} 0 & 0 & \mathrm{i} & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 & 0 \end{bmatrix} \qquad T_y = \begin{bmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & \mathrm{i} & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \end{bmatrix}. \tag{10}$$

These 4×4 translation matrices are again very special; they are such that for each lattice step the subspace of A_1 and B_2 symmetry is exchanged with the one of E_x and E_y symmetry, and

this means that we are about to obtain new $W = 0$ states. Indeed, $|\psi'^{(0)}_{A_1}\psi'^{(0)}_{B_2}\rangle_\sigma|\psi'^{(0)}_{E_x}\psi'^{(0)}_{E_y}\rangle_{-\sigma}$ is a four-body eigenstate of $\hat{W}$ with vanishing eigenvalue: under a lattice step translation this state does not change its spatial distribution but $\sigma \to -\sigma$. We may write that

$$|\psi'_{A_1}\psi'_{B_2}\rangle_\sigma|\psi'_{E_x}\psi'_{E_y}\rangle_{-\sigma} \longleftrightarrow |\psi'_{E_x}\psi'_{E_y}\rangle_\sigma|\psi'_{A_1}\psi'_{B_2}\rangle_{-\sigma} = |\psi'_{A_1}\psi'_{B_2}\rangle_{-\sigma}|\psi'_{E_x}\psi'_{E_y}\rangle_\sigma \tag{11}$$

and since ψ'_{A_1} is the only orbital having amplitude at $r = 0$ it is evident that this state has double occupation nowhere.

At this stage we have distinct local bases for both irreps of **G** having their basis vectors in $\mathcal{S}_{hf}$. From (7), (10) we see that under a lattice step translation the subspace spanned by $\{|\psi''^{(0)}_{A_1}\rangle, |\psi'^{(0)}_{A_1}\rangle, |\psi'^{(0)}_{B_2}\rangle\}$ is mapped onto the one spanned by $\{|\psi''^{(0)}_{B_1}\rangle, |\psi'^{(0)}_{E_x}\rangle, |\psi'^{(0)}_{E_y}\rangle\}$ and conversely. Now we are in position to get the exact ground state of the 4×4 square lattice for weak coupling. Consider the six-body determinantal eigenstate of the kinetic term H_0:

$$|\Phi_{AF}\rangle_\sigma = |\psi''^{(0)}_{A_1}\psi'^{(0)}_{A_1}\psi'^{(0)}_{B_2}\rangle_\sigma|\psi''^{(0)}_{B_1}\psi'^{(0)}_{E_x}\psi'^{(0)}_{E_y}\rangle_{-\sigma}. \tag{12}$$

In this state there is partial occupation of site $r = 0$ with spin σ, but no double occupation. A shift by a lattice step produces the transformation

$$|\Phi_{AF}\rangle_\sigma \longleftrightarrow -|\Phi_{AF}\rangle_{-\sigma}. \tag{13}$$

That is, a lattice step is equivalent to a spin flip, a feature that we call the *antiferromagnetic property*. Since the spin-flipped state is also free of double occupation, $|\Phi_{AF}\rangle_\sigma$ is a $W = 0$ eigenstate, and belongs to the first-order ground-state multiplet. Moreover, the single determinant with the antiferromagnetic property may be analysed in terms of its spin components, which must likewise be free of double occupation. We show below that there is at least one $W = 0$ state in $\mathcal{H}$ for each S. By Lieb's theorem, the unique ground state of the Hubbard model is the singlet component of (12); we shall deal with the projection in section 4.

We note that $|\psi''^{(0)}_{A_1}\rangle$ and $|\psi'^{(0)}_{A_1}\rangle$ are two one-particle states having non-vanishing occupation at $r = 0$, and we are getting a new one for each irrep of **G**; for some applications we might prefer having only one such state in $\mathcal{S}_{hf}$. This is easily accomplished after this preparation; we shall call the new local basis $|\varphi\rangle$. According to the above theorem, $\hat{n}_r$ has eigenvalues $3/8$ and (5 times) 0. For $r = 0$ the eigenvector of occupation $3/8$ is just the totally symmetric superposition of all of the $|k\rangle$ states in $\mathcal{S}_{hf}$; in terms of the eigenstates introduced above for the two-dimensional and four-dimensional irreps of **G**, we may write it in the form

$$|\varphi^{(0)}_1\rangle = \frac{1}{\sqrt{3}}|\psi''^{(0)}_{A_1}\rangle + \sqrt{\frac{2}{3}}|\psi'^{(0)}_{A_1}\rangle.$$

The above theorem also guarantees that the orthogonal linear combination of A_1 eigenstates of $n_{r=0}$:

$$|\varphi^{(0)}_2\rangle = \sqrt{\frac{2}{3}}|\psi''^{(0)}_{A_1}\rangle - \frac{1}{\sqrt{3}}|\psi'^{(0)}_{A_1}\rangle$$

has 0 eigenvalue. We are finished with the φ-basis, because the remaining local states are just eigenvectors with vanishing eigenvalue, and we may set

$$|\varphi^{(0)}_3\rangle = |\psi'^{(0)}_{B_2}\rangle \qquad |\varphi^{(0)}_4\rangle = |\psi''^{(0)}_{B_1}\rangle \qquad |\varphi^{(0)}_5\rangle = |\psi'^{(0)}_{E_x}\rangle \qquad |\varphi^{(0)}_6\rangle = |\psi'^{(0)}_{E_y}\rangle.$$

As anticipated, the $|\varphi\rangle$ local basis has the advantage that $|\varphi^{(0)}_1\rangle$ is the only element with non-zero occupation at $r = 0$; it also preserves the other useful properties that we have analysed

above. So the 6×6 translation matrix $(T_l)_{ij} = \langle \varphi_i^{(0)} | \varphi_j^{(\hat{e}_l)} \rangle$ is a *block-antidiagonal matrix*:

$$T_x = \begin{bmatrix} 0 & 0 & 0 & -1/\sqrt{3} & \mathrm{i}\sqrt{2/3} & 0 \\ 0 & 0 & 0 & -\sqrt{2/3} & -\mathrm{i}/\sqrt{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\mathrm{i} \\ -1/\sqrt{3} & -\sqrt{2/3} & 0 & 0 & 0 & 0 \\ \mathrm{i}\sqrt{2/3} & -\mathrm{i}/\sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} & 0 & 0 & 0 \end{bmatrix}$$

$$T_y = \begin{bmatrix} 0 & 0 & 0 & 1/\sqrt{3} & 0 & -\mathrm{i}\sqrt{2/3} \\ 0 & 0 & 0 & \sqrt{2/3} & 0 & \mathrm{i}/\sqrt{3} \\ 0 & 0 & 0 & 0 & \mathrm{i} & 0 \\ 1/\sqrt{3} & \sqrt{2/3} & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathrm{i} & 0 & 0 & 0 \\ -\mathrm{i}\sqrt{2/3} & \mathrm{i}/\sqrt{3} & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{14}$$

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

Indeed, $|\varphi_1^{(0)}\varphi_2^{(0)}\rangle$ is equivalent to $|\psi''^{(0)}_{\mathrm{A}_1}\psi'^{(0)}_{\mathrm{A}_1}\rangle$, because this is just a unitary transformation of the A_1 wave functions. Thus, we may write

$$|\Phi_{AF}\rangle_\sigma = |\varphi_1^{(0)}\varphi_2^{(0)}\varphi_3^{(0)}\rangle_\sigma |\varphi_4^{(0)}\varphi_5^{(0)}\varphi_6^{(0)}\rangle_{-\sigma}. \tag{15}$$

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 ξ 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 ξ 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.

3.4. The $N \times N$ square lattice for general even N

As discussed in section 3.2, we break $\mathcal{S}_{hf}$ into the bases of irreps of **G** that 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 $\hat{n}_r$ and Dirac's characters. For $N > 4$, $\mathcal{S}_{hf}$ contains k-vectors that do not possess any special symmetry and we get eight-dimensional irreps of **G** since the $R_i k$ are all different for all $R_i \in \mathrm{C}_{4\mathrm{v}}$. In other words, any eight-dimensional irrep of **G** is the regular representation of $\mathrm{C}_{4\mathrm{v}}$. Thus, by the Burnside theorem, it breaks into $\mathrm{A}_1 \oplus \mathrm{A}_2 \oplus \mathrm{B}_1 \oplus \mathrm{B}_2 \oplus \mathrm{E} \oplus \mathrm{E}$, with the two-dimensional irrep occurring twice; these are the symmetry labels of the local orbitals that we are looking for. Now let $k \in \mathcal{S}_{hf}$. The only eigenvector of the matrix $\langle R_i k | \hat{n}_{r=0} | R_j k \rangle$ corresponding to the non-vanishing eigenvalue λ relates to A_1. Let R_i, $i = 1, \ldots, 8$, denote respectively the identity **1**, the anticlockwise and clockwise 90° rotation $\mathrm{C}_4^{(+)}$, $\mathrm{C}_4^{(-)}$, the 180° rotation C_2, the reflections with respect to the $y = 0$ and $x = 0$ axes σ_x, σ_y, and the reflection with respect to the $x = y$ and $x = -y$ diagonals σ'_+, σ'_-. We can write down the eigenvectors of the above $n_{r=0}$ matrix as

$$|\psi_I^{(0)}\rangle = \sum_{i=1}^{8} O_{Ii} |R_i k\rangle$$

where $k_x \geqslant k_y \geqslant 0$ and O is the 8×8 orthogonal matrix

$$O = \frac{1}{\sqrt{8}} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 \end{bmatrix}. \tag{16}$$

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 $\langle R_i k|\hat{n}_r|R_j k\rangle$ and the Dirac characters of the point symmetry group. After very lengthy but elementary algebra one finds that the translation matrices $(T_l)_{JI} = \langle \psi_J^{(0)}|\psi_I^{(\hat{e}_l)}\rangle$ are

$$T_x = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cos k_x & \mathrm{i}\sin k_x & 0 \\ 0 & 0 & 0 & 0 & \cos k_x & 0 & 0 & -\mathrm{i}\sin k_x \\ 0 & 0 & 0 & 0 & 0 & \mathrm{i}\sin k_x & \cos k_x & 0 \\ 0 & 0 & 0 & 0 & \mathrm{i}\sin k_x & 0 & 0 & -\cos k_x \\ 0 & \cos k_x & 0 & \mathrm{i}\sin k_x & 0 & 0 & 0 & 0 \\ \cos k_x & 0 & \mathrm{i}\sin k_x & 0 & 0 & 0 & 0 & 0 \\ \mathrm{i}\sin k_x & 0 & \cos k_x & 0 & 0 & 0 & 0 & 0 \\ 0 & -\mathrm{i}\sin k_x & 0 & -\cos k_x & 0 & 0 & 0 & 0 \end{bmatrix} \tag{17}$$

and

$$T_y = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -\cos k_x & 0 & \bar{\mathrm{i}}\sin k_x \\ 0 & 0 & 0 & 0 & -\cos k_x & 0 & \mathrm{i}\sin k_x & 0 \\ 0 & 0 & 0 & 0 & \mathrm{i}\sin k_x & 0 & -\cos k_x & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathrm{i}\sin k_x & 0 & \cos k_x \\ 0 & -\cos k_x & \mathrm{i}\sin k_x & 0 & 0 & 0 & 0 & 0 \\ -\cos k_x & 0 & 0 & \mathrm{i}\sin k_x & 0 & 0 & 0 & 0 \\ 0 & \mathrm{i}\sin k_x & -\cos k_x & 0 & 0 & 0 & 0 & 0 \\ \bar{\mathrm{i}}\sin k_x & 0 & 0 & \cos k_x & 0 & 0 & 0 & 0 \end{bmatrix} \tag{18}$$

(we have used $\bar{\mathrm{i}} \equiv -\mathrm{i}$ twice to assist with layout) 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 a *block-antidiagonal form*; in particular they are such that the set containing the irreps A_1, B_2, E is mapped onto the set containing the irreps A_2, B_1, E′ and vice versa. This means that if we put four particles with spin σ in the former four irreps and four particles with spin $-\sigma$ in the latter four we obtain an eight-body state for which the translation by a lattice step is exactly equivalent to a spin flip (the *antiferromagnetic property*):

$$|\psi^{(0)}_{A_1}\psi^{(0)}_{B_2}\psi^{(0)}_{E_x}\psi^{(0)}_{E_y}\rangle_\sigma |\psi^{(0)}_{A_2}\psi^{(0)}_{B_1}\psi^{(0)}_{E'_x}\psi^{(0)}_{E'_y}\rangle_{-\sigma} \longleftrightarrow |\psi^{(0)}_{A_2}\psi^{(0)}_{B_1}\psi^{(0)}_{E'_x}\psi^{(0)}_{E'_y}\rangle_\sigma |\psi^{(0)}_{A_1}\psi^{(0)}_{B_2}\psi^{(0)}_{E_x}\psi^{(0)}_{E_y}\rangle_{-\sigma}. \tag{19}$$

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 σ does not have a partner of the same symmetry with spin $-\sigma$, the eight-body state of equation (19) cannot have double occupancy on any site and therefore it is a $W = 0$ state.

From now on we shall be engaged in 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

$|\psi^{(0)}\rangle \equiv |\psi\rangle$. 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 of the local orbitals of all of the irreps, half with spin up and half with spin down. Let $|\psi_I^{[m]}\rangle$ 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 mth 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

$$|\Phi_{AF}\rangle_\sigma \equiv \left|\left(\prod_{m=1}^{N_e} \psi_{A_1}^{[m]}\psi_{B_2}^{[m]}\psi_{E_x}^{[m]}\psi_{E_y}^{[m]}\right)\psi'_{A_1}\psi'_{B_2}\psi''_{A_1}\right\rangle_\sigma \times \left|\left(\prod_{m=1}^{N_e} \psi_{A_2}^{[m]}\psi_{B_1}^{[m]}\psi_{E'_x}^{[m]}\psi_{E'_y}^{[m]}\right)\psi'_{E_x}\psi'_{E_y}\psi''_{B_1}\right\rangle_{-\sigma} \tag{20}$$

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,

$$|\Phi_{AF}\rangle_\sigma \equiv \left|\left(\prod_{m=1}^{N_o} \psi_{A_1}^{[m]}\psi_{B_2}^{[m]}\psi_{E_x}^{[m]}\psi_{E_y}^{[m]}\right)\psi''_{A_1}\right\rangle_\sigma \left|\left(\prod_{m=1}^{N_o} \psi_{A_2}^{[m]}\psi_{B_1}^{[m]}\psi_{E'_x}^{[m]}\psi_{E'_y}^{[m]}\right)\psi''_{B_1}\right\rangle_{-\sigma}. \tag{21}$$

We can see from equations (8), (11), (19) 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 (the *antiferromagnetic property*). These results generalize equation (12). In both cases, the $-\sigma$-orbitals have $n_{r=0} = 0$, and the antiferromagnetic property guarantees that the states have $W = 0$. Equivalently, we could have obtained a generalized version of (15) by building a basis of symmetry-adapted eigenvectors of $\hat{n}_r$ for the whole set $\mathcal{S}_{hf}$, 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

$$P_S|\Phi_{AF}\rangle_\sigma \equiv |\Phi_{AF}^S\rangle_\sigma \neq 0 \qquad \forall S = 0, \ldots, N-1.$$

Then,

$$_\sigma\langle\Phi_{AF}|\hat{W}|\Phi_{AF}\rangle_\sigma = \sum_{S=1}^{N-1} {}_\sigma\langle\Phi_{AF}^S|\hat{W}|\Phi_{AF}^S\rangle_\sigma = 0$$

and this implies that there is at least one $W = 0$ state of $\hat{W}$ in $\mathcal{H}$ for each S. The ground state of H for weak coupling is the singlet $|\Phi_{AF}^0\rangle_\sigma$.

(2) The *existence* of this singlet $W = 0$ ground state is also a direct consequence of the Lieb theorem [13]. Indeed the maximum spin state $|\Phi_{AF}^{N-1}\rangle_\sigma$ is trivially in the kernel of $\hat{W}$; since the ground state must be a singlet it should be an eigenvector of $\hat{W}$ 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 that 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 for weak coupling.

(5) The ground-state interaction energy per site $E_U \equiv \langle\Phi_{AF}^0|\hat{W}|\Phi_{AF}^0\rangle/N^2$ can easily be evaluated with the help of equation (A.2). Since $|\Phi_{AF}^0\rangle$ belongs to the Hilbert space $\mathcal{H}$

and to the kernel of $\hat{W}$, E_U coincides with the shift (A.2) produced by the filled shells divided by N^2:

$$E_U = \frac{U}{N^4}\left[\frac{N^4}{4} - (N-1)^2\right] = \frac{U}{4} - U\frac{(N-1)^2}{N^4}. \tag{22}$$

This result tells us that in clusters the linear term of the expansion of the energy in powers of U is always smaller than the infinite-square-lattice value $U/4$.

(6) Finally we underline that in the state $|\Phi^0_{AF}\rangle$ only $2N-2$ particles are antiferromagnetically correlated while in the strong-coupling limit all the N^2 particles show antiferromagnetic correlations.

In the next section we study the symmetry properties of the singlet component of $|\Phi_{AF}\rangle_\sigma$.

4. 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 $\hat{S}^2$. 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 trying to find out the good quantum numbers of the ground state, the antisymmetric form

$$|\Phi_{AF}\rangle \equiv \frac{|\Phi_{AF}\rangle_\sigma - |\Phi_{AF}\rangle_{-\sigma}}{\sqrt{2}} \tag{23}$$

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.

4.1. Symmetry under translations

Equations (8), (11), (19) tell us that under a lattice step translation each of the determinantal states $|\Phi_{AF}\rangle_\sigma$ of equations (20), (21) 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 (23), $|\Phi_{AF}\rangle \to |\Phi_{AF}\rangle$ under a lattice step translation. Thus $|\Phi_{AF}\rangle$ is an eigenstate of the total momentum with eigenvalue $K_{tot} = (0,0)$. Since the spin projection cannot change this quantum number, it holds for $|\Phi^{S=0}_{AF}\rangle$ too.

4.2. Reflections and rotations

Now we study how $|\Phi_{AF}\rangle$ transforms under reflections and rotations with respect to the centre of an arbitrary plaquette of the square lattice. We are not compelled to refer the operations to the centre 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 reference [14].

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

$$R_i^{plaq} r = R_i(r - r_{plaq}) + r_{plaq}. \tag{24}$$

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

$$|k\rangle = \frac{1}{N}\sum_r \mathrm{e}^{-\mathrm{i}kr}|r\rangle \to |R_i^{plaq}k\rangle \equiv \frac{1}{N}\sum_r \mathrm{e}^{-\mathrm{i}kr}|R_i^{plaq}r\rangle = \mathrm{e}^{-\mathrm{i}k(r_{plaq}-R_i^{-1}r_{plaq})}|R_i k\rangle \tag{25}$$

where the last equality can be obtained with a change of variables. By means of equation (25) 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

$$|\psi''_{\mathrm{A}_1}\rangle = \frac{1}{\sqrt{2}}(|k_\mathrm{A}\rangle + |k_\mathrm{B}\rangle) \qquad |\psi''_{\mathrm{B}_1}\rangle = \frac{1}{\sqrt{2}}(|k_\mathrm{A}\rangle - |k_\mathrm{B}\rangle).$$

Under R_i^{plaq} we have

$$\begin{aligned} |\psi''_{\mathrm{A}_1}\rangle \to |R_i^{plaq}\psi''_{\mathrm{A}_1}\rangle &= \frac{1}{\sqrt{2}}(|R_i^{plaq}k_\mathrm{A}\rangle + |R_i^{plaq}k_\mathrm{B}\rangle) \\ |\psi''_{\mathrm{B}_1}\rangle \to |R_i^{plaq}\psi''_{\mathrm{B}_1}\rangle &= \frac{1}{\sqrt{2}}(|R_i^{plaq}k_\mathrm{A}\rangle - |R_i^{plaq}k_\mathrm{B}\rangle). \end{aligned} \tag{26}$$

The transformed *local* states $|R_i^{plaq}\psi''_I\rangle$, with $I = \mathrm{A}_1, \mathrm{B}_1$, can be expressed in terms of the original ones $|\psi''_I\rangle$:

$$|R_i^{plaq}\psi''_I\rangle = \sum_{J=\mathrm{A}_1,\mathrm{B}_1} |\psi''_J\rangle\langle\psi''_J|R_i^{plaq}\psi''_I\rangle. \tag{27}$$

Using equations (25) and computing the overlaps $\langle\psi''_J|R_i^{plaq}\psi''_I\rangle$ of equation (27), we have studied how the $W = 0$ pair state in equation (8) transforms under a 90° rotation $\mathrm{C}_4^{(+)}$ and reflection with respect to the $y = 0$ and $x = y$ axes, σ_x and σ'_+ respectively. After some algebra it is possible to show that

$$\begin{aligned} |\psi''_{\mathrm{A}_1}\rangle_\sigma|\psi''_{\mathrm{B}_1}\rangle_{-\sigma} &\longleftrightarrow -|\psi''_{\mathrm{B}_1}\rangle_\sigma|\psi''_{\mathrm{A}_1}\rangle_{-\sigma} && \mathrm{C}_4^{(+)} \\ |\psi''_{\mathrm{A}_1}\rangle_\sigma|\psi''_{\mathrm{B}_1}\rangle_{-\sigma} &\longleftrightarrow |\psi''_{\mathrm{B}_1}\rangle_\sigma|\psi''_{\mathrm{A}_1}\rangle_{-\sigma} && \sigma_x \\ |\psi''_{\mathrm{A}_1}\rangle_\sigma|\psi''_{\mathrm{B}_1}\rangle_{-\sigma} &\longleftrightarrow -|\psi''_{\mathrm{A}_1}\rangle_\sigma|\psi''_{\mathrm{B}_1}\rangle_{-\sigma} && \sigma'_+ \end{aligned} \tag{28}$$

where $\longleftrightarrow$ means that the left-hand side transforms into the right-hand side and conversely under the operation specified on the right.

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

$$|\Phi_{AF}\rangle = |\psi''_{\mathrm{A}_1}\rangle_\sigma|\psi''_{\mathrm{B}_1}\rangle_{-\sigma} + |\psi''_{\mathrm{B}_1}\rangle_\sigma|\psi''_{\mathrm{A}_1}\rangle_{-\sigma}. \tag{29}$$

By means of equations (28) 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 that the 2×2 case is special because $|\Phi_{AF}\rangle$ is already a singlet and thus must coincide with $|\Phi_{AF}^{S=0}\rangle$. This will no longer be true if $N \geqslant 4$.

Four-dimensional irrep. Similarly we can study the behaviour of the four-body $W = 0$ state of equation (11) under the three operations in equation (28). One finds

$$\begin{aligned} |\psi'_{\mathrm{A}_1}\psi'_{\mathrm{B}_2}\rangle_\sigma|\psi'_{\mathrm{E}_x}\psi'_{\mathrm{E}_y}\rangle_{-\sigma} &\longleftrightarrow -|\psi'_{\mathrm{E}_x}\psi'_{\mathrm{E}_y}\rangle_\sigma|\psi'_{\mathrm{A}_1}\psi'_{\mathrm{B}_2}\rangle_{-\sigma} && \mathrm{C}_4^{(+)} \\ |\psi'_{\mathrm{A}_1}\psi'_{\mathrm{B}_2}\rangle_\sigma|\psi'_{\mathrm{E}_x}\psi'_{\mathrm{E}_y}\rangle_{-\sigma} &\longleftrightarrow |\psi'_{\mathrm{E}_x}\psi'_{\mathrm{E}_y}\rangle_\sigma|\psi'_{\mathrm{A}_1}\psi'_{\mathrm{B}_2}\rangle_{-\sigma} && \sigma_x \\ |\psi'_{\mathrm{A}_1}\psi'_{\mathrm{B}_2}\rangle_\sigma|\psi'_{\mathrm{E}_x}\psi'_{\mathrm{E}_y}\rangle_{-\sigma} &\longleftrightarrow -|\psi'_{\mathrm{A}_1}\psi'_{\mathrm{B}_2}\rangle_\sigma|\psi'_{\mathrm{E}_x}\psi'_{\mathrm{E}_y}\rangle_{-\sigma} && \sigma'_+. \end{aligned} \tag{30}$$

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

$$|\Phi_{AF}\rangle = |\psi'_{A_1}\psi'_{B_2}\psi''_{A_1}\rangle_\sigma|\psi'_{E_x}\psi'_{E_y}\psi''_{B_1}\rangle_{-\sigma} + |\psi'_{E_x}\psi'_{E_y}\psi''_{B_1}\rangle_\sigma|\psi'_{A_1}\psi'_{B_2}\psi''_{A_1}\rangle_{-\sigma}. \tag{31}$$

Using equations (28) and (30) 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 eight-dimensional irrep of **G** contained in $\mathcal{S}_{hf}$.

Eight-dimensional irrep. After very lengthy but simple algebra we have found that the eight-body state of equation (19) transforms as

$$\begin{aligned}
&|\psi_{A_1}\psi_{B_2}\psi_{E_x}\psi_{E_y}\rangle_\sigma|\psi_{A_2}\psi_{B_1}\psi_{E'_x}\psi_{E'_y}\rangle_{-\sigma} \longleftrightarrow |\psi_{A_2}\psi_{B_1}\psi_{E'_x}\psi_{E'_y}\rangle_\sigma|\psi_{A_1}\psi_{B_2}\psi_{E_x}\psi_{E_y}\rangle_{-\sigma} \qquad C_4^{(+)}\\
&|\psi_{A_1}\psi_{B_2}\psi_{E_x}\psi_{E_y}\rangle_\sigma|\psi_{A_2}\psi_{B_1}\psi_{E'_x}\psi_{E'_y}\rangle_{-\sigma} \longleftrightarrow |\psi_{A_2}\psi_{B_1}\psi_{E'_x}\psi_{E'_y}\rangle_\sigma|\psi_{A_1}\psi_{B_2}\psi_{E_x}\psi_{E_y}\rangle_{-\sigma} \qquad \sigma_x\\
&|\psi_{A_1}\psi_{B_2}\psi_{E_x}\psi_{E_y}\rangle_\sigma|\psi_{A_2}\psi_{B_1}\psi_{E'_x}\psi_{E'_y}\rangle_{-\sigma} \longleftrightarrow |\psi_{A_1}\psi_{B_2}\psi_{E_x}\psi_{E_y}\rangle_\sigma|\psi_{A_2}\psi_{B_1}\psi_{E'_x}\psi_{E'_y}\rangle_{-\sigma} \qquad \sigma'_+.
\end{aligned} \tag{32}$$

For $k_x \to \pi/2$ the eight-dimensional irrep is equivalent to two four-dimensional ones and the equations (32) are the 'squares' of the equations (30). Analogously for $k_x \to \pi$ we obtain four times the two-dimensional irrep and equations (32) are the 'fourth powers' of equations (28).

From (32) we deduce that whatever the number of eight-dimensional irreps, the symmetry of $|\Phi_{AF}\rangle$ depends only by the presence or absence of the four-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 $|\Phi_{AF}^{S=0}\rangle$ 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 reference [14] 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 for weak and strong coupling.

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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 $\binom{2N-2}{N-1}^2$ 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 $\hat{W}$-matrix over such a basis.

The diagonal elements of the $\hat{W}$-matrix are just expectation values over determinants $|k_\alpha\uparrow k_\beta\downarrow\cdots\rangle$. Such an expectation value is a sum over all of the possible pairs of the bielectronic

elements of $\hat{W}$ like

$$W(\alpha\beta,\alpha\beta) = \sum_r U\langle k_\alpha|n_r|k_\alpha\rangle\langle k_\beta|n_r|k_\beta\rangle$$
$$= \sum_r U\frac{1}{N^2}e^{i(k_\alpha-k_\alpha)r}\frac{1}{N^2}e^{i(k_\beta-k_\beta)r} = \frac{U}{N^4}N^2 = \frac{U}{N^2}. \tag{A.1}$$

The result is independent of k_α and k_β. 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 $UN^2/4$.

The off-diagonal elements of the $\hat{W}$-matrix connecting determinants that differ by three or more spin orbitals vanish because $\hat{W}$ is a two-body operator. The off-diagonal elements connecting determinants that differ by one spin orbital are sums of contributions like

$$W(\alpha\beta,\gamma\beta) = \sum_r U\langle k_\alpha|n_r|k_\gamma\rangle\langle k_\beta|n_r|k_\beta\rangle$$

that vanish because of the orthogonality of the plane-wave orbitals. One is left with the off-diagonal elements connecting determinants that differ by two spin orbitals, which coincide with the corresponding bielectronic elements

$$W(\alpha\beta,\gamma\delta) = \sum_r U\langle k_\alpha|n_r|k_\gamma\rangle\langle k_\beta|n_r|k_\delta\rangle.$$

These are just the off-diagonal matrix elements of $\hat{W}$ over the truncated Hilbert space $\mathcal{H}$ spanned by the states of the holes in the half-filled shell, ignoring the filled ones. Thus the only effect of the filled shells is to shift all the eigenvalues of the $\hat{W}$-matrix over the Hilbert space $\mathcal{H}$ by a fixed amount given by

$$\frac{U}{N^2}\left[\frac{N^4}{4} - (N-1)^2\right]. \tag{A.2}$$

We stress that there are $N-1$ holes of each spin in $\mathcal{S}_{hf}$ and 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 (5). Expanding the determinant according to its definition in terms of the totally antisymmetric tensor ϵ:

$$\det|(n_r)_{ij} - \lambda\delta_{ij}| = \sum_{i_1\cdots i_{|\mathcal{S}|}} \epsilon_{i_1\cdots i_{|\mathcal{S}|}}\left(\frac{1}{N^2}e^{i(k_1-k_{i_1})r} - \lambda\delta_{1,i_1}\right)\cdots\left(\frac{1}{N^2}e^{i(k_{|\mathcal{S}|}-k_{i_{|\mathcal{S}|}})r} - \lambda\delta_{|\mathcal{S}|,i_{|\mathcal{S}|}}\right) \tag{B.1}$$

we see that the term of maximum order in λ 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 λ is the sum of $|\mathcal{S}|$ identical contributions also arising from the fundamental permutation. Therefore, it is

$$\frac{|\mathcal{S}|}{N^2}(-\lambda)^{|\mathcal{S}|-1}. \tag{B.2}$$

It is not difficult to see that all of the other orders in λ yield nothing. At order zero one finds

$$\frac{1}{N^{2|\mathcal{S}|}}\sum_{i_1\cdots i_{|\mathcal{S}|}} \epsilon_{i_1\cdots i_{|\mathcal{S}|}}e^{i(k_1+\cdots+k_{|\mathcal{S}|}-k_{i_1}-\cdots-k_{i_{|\mathcal{S}|}})r}. \tag{B.3}$$

Since the exponential is totally symmetric in the permutation of $i_1 \cdots i_{|\mathcal{S}|}$ while ϵ is totally antisymmetric, the sum vanishes.

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

$$\frac{1}{N^{2(|\mathcal{S}|-1)}} \sum_{i_2 \cdots i_{|\mathcal{S}|}} \epsilon_{1 i_2 \cdots i_{|\mathcal{S}|}} \mathrm{e}^{\mathrm{i}(k_2 + \cdots + k_{|\mathcal{S}|} - k_{i_2} - \cdots - k_{i_{|\mathcal{S}|}})r}. \tag{B.4}$$

Again, the exponential is symmetric: $i_2 \cdots i_{|\mathcal{S}|}$ and the sum in equation (B.4) vanish. Clearly, this argument applies to all of the contributions to first order and to all orders less than $|\mathcal{S}| - 1$.

So, we are left with only two non-vanishing terms:

$$\det|n_r - \lambda| = (-\lambda)^{|\mathcal{S}|-1}\left(\frac{|\mathcal{S}|}{N^2} - \lambda\right). \tag{B.5}$$

That is, we have obtained equation (5).

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[3]

$$|\Psi\rangle_\sigma \equiv |\psi_1 \cdots \psi_n\rangle_\sigma |\psi_{n+1} \cdots \psi_{2n}\rangle_{-\sigma} \tag{C.1}$$

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 not an eigenstate of $\hat{S}^2$ 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 [20]:

i_1	i_2	$\cdots$	i_{n-S}	i_{n-S+1}	$\cdots$	i_{n+S}
j_1	j_2	$\cdots$	j_{n-S}			

(C.2)

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 with the above table the operator

$$\prod_{a=1}^{n+S-1}\left(1 + \sum_{\alpha=1}^{n+S-a} C_{i_\alpha, i_{n+S-a+1}}\right) \prod_{b=1}^{n-S-1}\left(1 + \sum_{\beta=1}^{n-S-b} C_{j_\beta, j_{n-S-b+1}}\right) \prod_{l=1}^{n-S}(1 - C_{i_l, j_l}). \tag{C.3}$$

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

Example:

$$n = 2 \Longrightarrow |\Psi\rangle_\sigma = |\psi_1 \uparrow \psi_2 \uparrow \psi_3 \downarrow \psi_4 \downarrow\rangle \equiv |\psi_1 \psi_2\rangle_\uparrow |\psi_3 \psi_4\rangle_\downarrow.$$

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

In this case the three projection operators are

$$P_{S=2} \propto \begin{array}{|c|c|c|c|}\hline 1&2&3&4\\\hline\end{array}$$

$$P_{S=1} \propto \begin{array}{|c|c|c|}\hline 1&2&3\\\hline 4\\\cline{1-1}\end{array} + \begin{array}{|c|c|c|}\hline 1&2&4\\\hline 3\\\cline{1-1}\end{array} + \begin{array}{|c|c|c|}\hline 1&3&4\\\hline 2\\\cline{1-1}\end{array} \tag{C.4}$$

$$P_{S=0} \propto \begin{array}{|c|c|}\hline 1&2\\\hline 3&4\\\hline\end{array} + \begin{array}{|c|c|}\hline 1&3\\\hline 2&4\\\hline\end{array}\,.$$

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:

$$P_{S=0} = \begin{array}{|c|c|c|c|}\hline 1&2&\cdots&n\\\hline n+1&n+2&\cdots&2n\\\hline\end{array}\,. \tag{C.5}$$

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.

References

[1] Bednorz J G and Müller K A 1986 *Z. Phys.* B **64** 188
[2] Monthoux P and Scalapino D J 1994 *Phys. Rev. Lett.* **72** 1874
[3] Vilk Y M and Tremblai A-M S 1997 *Preprint* cond-mat/9702188
[4] Zanchi D and Schulz H J 1996 *Phys. Rev.* B **54** 9509
[5] Halboth C J and Metzner W 1999 *Preprint* cond-mat/9908471
[6] Fano G, Ortolani F and Parola A 1990 *Phys. Rev.* B **42** 6877
[7] Cini M and Balzarotti A 1997 *Phys. Rev.* B **56** 14 711
[8] Fettes W and Morgensten I 1999 *Eur. Phys.* B **9** 635
[9] Anderson P W 1959 *Phys. Rev.* **115** 2
[10] Gutzwiller M C 1963 *Phys. Rev. Lett.* **10** 159
[11] Galan J and Verges J A 1991 *Phys. Rev.* B **44** 10 093
[12] Metzner W and Vollhardt D 1989 *Phys. Rev.* B **39** 4462
[13] Lieb E H 1989 *Phys. Rev. Lett.* **62** 1201
[14] Moreo A and Dagotto E 1990 *Phys. Rev.* B **41** 9488
[15] Cini M, Perfetto E and Stefanucci G 2001 to be published
[16] Hamermesh M 1962 *Group Theory and its Application to Physical Problems* (Reading, MA: Addison-Wesley)
[17] Cini M, Balzarotti A, Brunetti R, Gimelli M and Stefanucci G 2001 *Int. J. Mod. Phys.* at press
[18] Cini M, Stefanucci G and Balzarotti A 1999 *Solid State Commun.* **109** 229
[19] Cini M, Stefanucci G and Balzarotti A 1999 *Euro. Phys. J.* B **10** 293
[20] Greiner W and Müller B 1989 *Quantum Mechanics—Symmetries* (Berlin: Springer)