Analytic Correlation Functions of the two-dimensional Half Filled
Hubbard Model at Weak Coupling

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We derive explicit spin and charge correlation functions of the \( N \times N \) Hubbard model from a recently obtained weak-coupling analytic ground state \( |\Psi_{\text{AF}}^{(0)}\rangle \). The spin correlation function shows an antiferromagnetic behaviour with different signs for the two sublattices and its Fourier transform is peaked at \( Q = (\pi, \pi) \). The charge correlation function presents two valleys at 45 degrees from the axes. Both functions behave in a smooth way with increasing \( N \); the results agree well with the available numerical data.

I. INTRODUCTION

Let us consider the Hubbard model with hamiltonian

\[
H = H_0 + \hat{W} = t \sum_{\sigma} \sum_{(r,r')} c_{r,\sigma}^\dagger c_{r',\sigma} + \sum_{r} U n_{r,\uparrow} n_{r,\downarrow}, \quad U > 0,
\]

on a bipartite square lattice \( \Lambda = \mathcal{A} \cup \mathcal{B} \) 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 \( (r, r') \) is over the pairs of nearest neighbor sites and \( \hat{n}_{r,\sigma} \) is the number operator on site \( r \) of spin \( \sigma \). The point symmetry is \( C_{4v} \), the Group of a square\(^1\); besides, \( H \) is invariant under the commutative Group of Translations \( T \) and hence under the Space Group \( G = T \otimes C_{4v}; \otimes \) means the semidirect product. The presence of spin and pseudospin symmetries [1] leads to \( S O_4 \) Group [2] [3]; below, we shall work in the subspace of vanishing spin and pseudospin. We represent sites by \( r = (x,y) \) and wave vectors by \( k = (k_x,k_y) = \frac{2\pi}{\Lambda}(x,y) \), with \( x,y = 0,\ldots, N - 1 \). In terms of the Fourier expanded fermion operators \( c_{k,\sigma} = \frac{1}{N} \sum_{r} e^{ik \cdot r} c_{r,\sigma} \), 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 \( H_0 \).

The \( N \times N \) Hubbard model at half filling is not elementary, even in the innocent-looking case of finite \( N \) and small repulsion \( U \). Indeed, weak-coupling expansions have long been known to be highly informative [4], [5]. The reason is that the trivial \( U = 0 \) case is \( \left( \frac{2N - 2}{N - 1} \right)^2 \) times degenerate, and so even for relatively small lattices one has to solve a big secular problem to see how the interaction resolves the degeneracy in first-order. To deal with this problem, recently [6] [7] we have proposed a local formalism, based on diagonalizing the occupation number operators in the degenerate eigenstates of the kinetic energy \( H_0 \). We came out with an analytic singlet wave function \( |\Psi_{\text{AF}}^{(0)}\rangle \) which solves the secular problem and belongs to the ground eigenvalue of \( H \). Under a lattice step translation it just flips spins (antiferromagnetic property). Further we proved that

\(^1\)\( C_{4v} \) 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 | 2 | \( C_{4v}^{(+)} \) | \( C_{4v}^{(-)} \) |
|---|---|---|---|---|
| \( A_1 \) | 1 | 1 | 1 | 1 |
| \( A_2 \) | 1 | -1 | -1 | -1 |
| \( B_1 \) | 1 | 1 | -1 | -1 |
| \( B_2 \) | 1 | -1 | 1 | 1 |
| \( E \) | 2 | -2 | 0 | 0 |
it has vanishing momentum and its point symmetry is the same as the ground state symmetry established by Moreo and Dagotto [8].

We believe that \( |\psi_{AF}^0\rangle \) clearly deserves further study: although it is an eigenstate only at the first order in \( U \), it must represent a good deal of the properties of the full ground state. Here we wish to show that the same local formalism that allows one to build \( |\psi_{AF}^0\rangle \), is also suitable to bring out some physics. It is clear that the importance of analytic results is actually enhanced in the age of computers, since they can benchmark the numerical approximations.

The correlation functions are a popular tool to understand and visualize the structure and the physical properties of a given many-body state. The definitions are:

\[
G_{\text{charge}}(\mathbf{r}) \equiv \langle \psi_{AF}^0 | \hat{n}_r \hat{n}_0 | \psi_{AF}^0 \rangle, \tag{2}
\]

for the charge correlation function and

\[
G_{\text{spin}}(\mathbf{r}) \equiv \langle \psi_{AF}^0 | \hat{S}_r \cdot \hat{S}_0 | \psi_{AF}^0 \rangle. \tag{3}
\]

for the spin one. Here \( \hat{n}_r \) is the number operator and \( \hat{S}_r \) is the spin vector operator at site \( \mathbf{r} \); the pedices 0 denote the site at the origin.

Studies [9] of correlation functions in the three-band Hubbard model have been aimed to the characterization of possible pairing mechanisms short after the discovery of high-\( T_c \) superconductivity [10]. Much of the early work dealt with the one-band model at strong coupling. Let us mention the exact diagonalization study by Kaxiras and Manousakis [11] on the \( \sqrt{10} \times \sqrt{10} \) lattice, showing the antiferromagnetic order at half filling; the diagrammatic approach by Gebhard and Vollhardt [12] used the Gutzwiller ansatz, mainly for the 1d chain. Correlation functions on larger lattices of the one-band [13], and, more recently, of the three-band Hubbard Model [14] [15] have been obtained by Quantum-Monte-Carlo methods. They have also been used to benchmark the self-consistent theory by Vilk et al. [16], which is basically a generalized Random-Phase Approximation.

After summarizing the local formalism and the ground state solution in Section II, we go over in Section III to a new picture by a particle-hole canonical transformation which is convenient to calculate the correlation functions. We derive the spin correlation function in Section IV and the charge one in Section V. The results are discussed and compared with available data in Section VI.

\section{II. THE GROUND STATE AT WEAK COUPLING}

In order to establish some notations we need to review the ground state formalism [6], [7]. Let \( \mathcal{S}_{hf} \) denote the set (or shell) of the \( \mathbf{k} \) wave vectors such that \( \epsilon(\mathbf{k}) = 0 \). At half filling (\( N^{2} \) particles) for \( U = 0 \) the \( \mathcal{S}_{hf} \) shell is half occupied, while all \( |\mathbf{k}\rangle \) orbitals such that \( \epsilon(\mathbf{k}) < 0 \) are filled. The \( \mathbf{k} \) 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,

\[
\hat{S}^z = \frac{1}{2} \sum_{\mathbf{r}} (\hat{n}_r^\uparrow - \hat{n}_r^\downarrow), \quad \hat{S}^+ = \sum_{\mathbf{r}} c_{\mathbf{r}}^\dagger c_{\mathbf{r}+\mathbf{1}}, \quad \hat{S}^- = (\hat{S}^+)^\dagger,
\]

at half filling every ground state of \( H_0 \) is represented in the \( \hat{S}^z = 0 \) subspace. Thus, \( H_0 \) has \( \left( \frac{2N - 2}{N - 1} \right)^2 \) degenerate unperturbed ground state configurations with \( \hat{S}^z = 0 \).

It can be shown [6] 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 \( \mathcal{S}_{hf} \). 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 emphasize 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 large set \( \mathcal{S}_{hf} \) breaks into small pieces if we take full advantage of the \( \mathbf{G} \) symmetry. Any plane-wave state \( \mathbf{k} \) belongs to a one-dimensional irrep of \( \mathbf{T} \); moreover, it also belongs to a star of \( \mathbf{k} \) 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 \( \mathbf{k} \in \mathcal{S}_{hf} \) lies on a square with vertices on the axes at the Brillouin zone boundaries. Choosing an arbitrary \( \mathbf{k} \in \mathcal{S}_{hf} \) with \( k_x \geq k_y \geq 0 \), hence \( k_x + k_y = \pi \), the set of vectors \( R_i \mathbf{k} \in \mathcal{S}_{hf} \), where \( R_i \in C_{4v} \), is a basis for an irrep of \( \mathbf{G} \). The high symmetry vectors \( \mathbf{k}_A = (\pi, 0) \) and \( \mathbf{k}_B = (0, \pi) \) are the basis of the only two-dimensional irrep of \( \mathbf{G} \), which exists for any \( N \). If \( N/2 \) is even, one also finds the high symmetry wavevectors \( \mathbf{k} = (\pm \pi/2, \pm \pi/2) \) which mix among themselves under \( C_{4v} \) operations and yield a four-dimensional irrep. In general, when \( \mathbf{k} \) is not in a
special symmetry direction, the vectors $R_i \mathbf{k}$ 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 + 4 times that of four-dimensional ones + 2 for the only two-dimensional irrep must yield $|S_{E_4}| = 2N - 2$, one finds that $S_{E_4}$ contains $N = \frac{1}{2}(\frac{N}{2} - 2)$ irreps of dimension 8 if $N/2$ is even and $N = \frac{1}{2}(\frac{N}{2} - 1)$ irreps of dimension 8 if $N/2$ is odd.

In this way, $S_{E_4}$ is seen to be the union of disjoint bases of irreps of the Space Group. This break-up of $S_{E_4}$ enables us to define a real symmetry adapted one-body local basis which allows to carry on the analysis for any $N$.

The one-body local basis is obtained by projecting onto the irreps of $C_{4v}$ the $\mathbf{k}$ states of $S_{E_4}$ that belong to a given irrep of $G$. As already noted, $\mathbf{k}_A = (\pi, 0)$ and $\mathbf{k}_B = (0, \pi)$ belong to $S_{E_4}$ and are the basis of a two-dimensional irrep of $G$. Let

$$|\psi_{A_i}\rangle = \frac{1}{\sqrt{2}}(|\mathbf{k}_A\rangle + |\mathbf{k}_B\rangle), \quad |\psi_{B_i}\rangle = \frac{1}{\sqrt{2}}(|\mathbf{k}_A\rangle - |\mathbf{k}_B\rangle)$$

be the first two real states of the local basis. As the notation implies, both are simultaneously eigenvectors of the Dirac characters of $C_{4v}$, and carry symmetry labels; actually the symmetries are $A_1$ and $B_1$ because the two-dimensional irrep of $G$ breaks into $A_1 \oplus B_1$ in $C_{4v}$. In $G$ these two functions merge into one irrep because the $\mathbf{k}$ states pick up phase factors from the translations.

For even $N/2$, $S_{h_4}$ also comprises the basis wave vectors $\mathbf{k}_1 = (\pi/2, \pi/2)$, $\mathbf{k}_2 = (-\pi/2, \pi/2)$, $\mathbf{k}_3 = (\pi/2, -\pi/2)$, $\mathbf{k}_4 = (-\pi/2, -\pi/2)$ of the 4-dimensional irrep of $G$. This irrep breaks into $A_1 \oplus B_2 \oplus E$ in $C_{4v}$. Letting $I = 1, 2, 3, 4$ for the irreps $A_1$, $B_2$, $E_x$, $E_y$ respectively, we can write down four more real local states

$$|\psi_I\rangle = \sum_{i=1}^{4} O'_i |\mathbf{k}_i\rangle,$$

where $O'$ is the $4 \times 4$ unitary matrix which performs the projections, namely,

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

For $N > 4$, $S_{h_4}$ also contains $\mathbf{k}$ vectors that are away from special symmetry directions. These form eight-dimensional irreps of $G$ since $R_i \mathbf{k}$ are all different for all $R_i \in C_{4v}$. 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. Let $\mathbf{k}^{[m]} = (k_x^{[m]}, k_y^{[m]})$ with $k_x^{[m]} \geq k_y^{[m]} \geq 0$ be a wave vector of the $m$-th eight dimensional irrep of $G$ and let $R_i, i = 1, \ldots, 8$ denote respectively the identity $1$, the counterclockwise and clockwise 90 degrees rotation $C_4^{(\pm)}$, $C_4^{(-)}$, 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 $\sigma'_x$, $\sigma'_y$. We write down real local basis states as

$$|\psi_{Ii}\rangle = \sum_{i=1}^{8} O_i |R_i \mathbf{k}^{[m]}\rangle,$$

where $O$ is the $8 \times 8$ unitary matrix

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

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.
Now let us consider the following determinantal state

$$|\Phi_{AF}\rangle_\sigma \equiv \prod_{m=1}^{N_e} \psi_{A_1}^{[m]} \psi_{B_2}^{[m]} \psi_{B_2}^{[m]} \psi_{B_1}^{[m]} \left( \psi_{A_1}^{[m]} \psi_{B_2}^{[m]} \psi_{B_2}^{[m]} \psi_{B_1}^{[m]} \right)^\sigma \otimes \left( \prod_{m=1}^{N_e} \psi_{A_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_1}^{[m]} \right)^\sigma' \psi_{E_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_1}^{[m]} \psi_{E_1}^{[m]} \psi_{E_1}^{[m]} \psi_{E_1}^{[m]} - \sigma' \right),$$

(10)

for even \(N/2\) and

$$|\Phi_{AF}\rangle_\sigma \equiv \left( \prod_{m=1}^{N_e} \psi_{A_1}^{[m]} \psi_{B_2}^{[m]} \psi_{B_2}^{[m]} \psi_{B_1}^{[m]} \right)^\sigma \otimes \left( \prod_{m=1}^{N_e} \psi_{A_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_1}^{[m]} \right)^\sigma' \psi_{E_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_2}^{[m]} \psi_{E_1}^{[m]} \psi_{E_1}^{[m]} \psi_{E_1}^{[m]} \psi_{E_1}^{[m]} - \sigma' \right),$$

(11)

for odd \(N/2\), with \(\sigma = \uparrow, \downarrow\). In Ref. [6] [7] we have shown that

- \(|\Phi_{AF}\rangle_\sigma\) is an eigenstate of \(\hat{W}\) with vanishing eigenvalue (\(W = 0\) state).
- Under a lattice step translation \(|\Phi_{AF}\rangle_\sigma \rightarrow -|\Phi_{AF}\rangle_{-\sigma}\). Therefore, it manifestly shows an antiferromagnetic order (antiferromagnetic property).
- Introducing the projection operator \(P_S\) on the spin \(S\) subspace, one finds that \(P_S|\Phi_{AF}\rangle_{\sigma} \equiv \Phi_{AF}^{[S]} \neq 0, \forall S = 0, \ldots, N - 1\). Then, \(|\Phi_{AF}\rangle|\Phi_{AF}\rangle = \sum_{S=0}^{N-1} (\Phi_{AF}^{[S]}|\Phi_{AF}^{[S]}\rangle = 0, and this implies that there is at least one \(W = 0\) state of \(\hat{W}\) in \(\mathcal{H}\) for each \(S\). By the Lieb Theorem [1], only the singlet component \(|\Phi_{AF}^{[0]}\rangle\) belongs to the ground state multiplet of \(H\) at weak coupling (filled shells are understood, of course).
- \(|\Phi_{AF}^{[0]}\rangle\) has vanishing total momentum, is even under reflections, while the point symmetry is \(s\) or \(d\) for even or odd \(N/2\), respectively. These are the correct quantum numbers of the interacting ground state at half filling [8].
- The ground state interaction energy per site is

$$E_U \equiv \left( |\Phi_{AF}^{[0]}\rangle|\hat{W}|\Phi_{AF}^{[0]}\rangle \right) / N^2 = \frac{U}{4} - \frac{U (N - 1)^2}{N^4}.$$  

(12)

Thus the linear term of the expansion of the energy per site in powers of \(U\) increases monotonically with \(N\) towards the infinite square lattice value \(U/4\).

Finally we emphasize that in \(|\Phi_{AF}^{[0]}\rangle\) only \(2N - 2\) particles are antiferromagnetically correlated while in the strong coupling limit all the \(N^2\) show antiferromagnetic correlations.

\(|\Phi_{AF}^{[0]}\rangle\) is an exact ground state of \(H\) for \(U \to 0\). Does this mean that it is the \(U \to 0\) limit of the unique interacting ground state? We know that this is the case for the \(4 \times 4\) and \(6 \times 6\) square lattices, where we have numerical evidence that \(|\Phi_{AF}^{[0]}\rangle\) is the only singlet eigenstate in \(\mathcal{H}\) with vanishing eigenvalue. The correlation functions that we find below behave quite reasonably also for \(N > 6\) and this strongly suggests that \(|\Phi_{AF}^{[0]}\rangle\) continues to be a good approximation to the true ground state at weak coupling. A proof of the uniqueness of the vanishing eigenvalue of \(\hat{W}\) in the singlet subspace of \(\mathcal{H}\) would be sufficient (although not necessary) to prove that. In the next Section we find further evidence to support this proposal: we write \(|\Phi_{AF}^{[0]}\rangle\) in the particle-hole transformed picture and show that the corresponding Lieb matrix is positive semidefinite, as it should be for a genuine ground state [1].

### III. THE GROUND STATE IN THE PARTICLE-HOLE TRANSFORMED PICTURE

The unitary particle-hole transformation on a square \(N \times N\) lattice and even \(N\) reads

$$\begin{cases} c_{r\uparrow} = d_{r\downarrow}, \\ c_{r\downarrow} = (-)^{x+y} d_{r\uparrow}, \end{cases} \quad r = (x, y).$$

(13)

This transformation maps the repulsive Hubbard model described in Eq.(1) onto the attractive one

$$H = t \sum_{\sigma} \sum_{(r,r')} d_{r\sigma}^\dagger d_{r'\sigma} - \sum_{r} U \hat{n}^{(d)}_{r\uparrow} \hat{n}^{(d)}_{r\downarrow} + U \hat{n}^{(d)}_{r\uparrow}, \quad U > 0,$$

(14)
Let $\hat{a}_n^{(d)} = d_n^\dagger d_n$ and $\hat{N}_n^{(d)} = \sum_n \hat{a}_n^{(d)}$. Letting $|\Psi_{\Gamma}\rangle$ be an orthonormal real basis of $N^2/2$-particle states (that is, each $|\Psi_{\Gamma}\rangle$ must be an homogeneous polynomial of degree $N^2/2$ in the $d_n^\dagger$ with real coefficients acting on the vacuum), we remind that the ground state at half filling

$$|\Psi^{[\text{0}]\rangle} = \sum_{\Gamma_1,\Gamma_2} L_{\Gamma_1,\Gamma_2} |\Psi_{\Gamma_1\uparrow}\rangle \otimes |\Psi_{\Gamma_2\downarrow}\rangle$$

(15)

is such that the Lieb matrix $L_{\Gamma_1,\Gamma_2}$ is positive (or negative) semidefinite.

In this Section we will perform the unitary particle-hole transformation in Eq.(13) on the ground state of Eqs.(10)(11). We will show that the corresponding Lieb matrix is indeed positive semidefinite; besides, it is already diagonal in the local basis. As a consequence, the ground state in the untransformed $(c)$ picture is a pseudospin (as well as spin) singlet.

Let $c_i^\dagger$, $i = 1, \ldots, 2N - 2$, be the operators which create a particle in the $i$-th local state contained in $|\Phi_{AF}\rangle$, Eqs.(10)(11). We write $|\Phi_{AF}\rangle_\sigma$ as

$$|\Phi_{AF}\rangle_\sigma = c_1^\dagger \cdots c_{N-1,\sigma}^\dagger c_{N,-\sigma}^\dagger \cdots c_{2N-2,-\sigma}^\dagger |0\rangle.$$  

(16)

It is clear that the first [last] $N - 1$ creation operators refer to the states of spin $\sigma [-\sigma]$ in Eqs.(10)(11). The singlet projection gives

$$|\Phi^{[0]}_{AF}\rangle = P_{S=0} |\Phi_{AF}\rangle_\uparrow = \frac{1}{\sqrt{N}} \sum_{k=N/2}^{N-1} (-)^{k} g_k \sum_{i_1 \cdots i_{N/2}} \hat{S}_{i_1}^+ \cdots \hat{S}_{i_{N/2}}^+ \{ \hat{S}_{j_1}^- \cdots \hat{S}_{j_{N/2}}^- [ \hat{S}_{j_1}^+ \cdots \hat{S}_{j_{N/2}}^+ ] \} \times$$

$$\times c_{i_1,\uparrow}^\dagger \cdots c_{i_{N/2},\uparrow}^\dagger c_{j_1,\downarrow}^\dagger \cdots c_{j_{N/2},\downarrow}^\dagger |0\rangle + \frac{1}{\sqrt{N}} \sum_{k=N/2}^{N-1} (-)^{k+1} g_k \sum_{i_1 \cdots i_{N/2}} \hat{S}_{i_1}^- \cdots \hat{S}_{i_{N/2}}^- \{ \hat{S}_{j_1}^+ \cdots \hat{S}_{j_{N/2}}^+ [ \hat{S}_{j_1}^- \cdots \hat{S}_{j_{N/2}}^- ] \} \times$$

$$\times c_{i_1,\downarrow}^\dagger \cdots c_{i_{N/2},\downarrow}^\dagger c_{j_1,\uparrow}^\dagger \cdots c_{j_{N/2},\uparrow}^\dagger |0\rangle$$

(17)

where $\hat{S}_i^+ = c_{i,\uparrow}^\dagger c_{i,\downarrow}$, $\hat{S}_i^- = (\hat{S}_i^+)^\dagger$, $N$ is the normalization constant

$$N = 2 \left[ \sum_{k=1}^{N/2} g_k^2 \left( \frac{N-1}{N/2-k} \right)^2 \right].$$

(18)

and the $g_k$'s are given by

$$g_k = \left( \frac{N/2 + k - 1}{N/2 - 1} \right) \left( \frac{N/2 - k}{N/2 - k} \right).$$

(19)

Let

$$c_k = \frac{1}{N} \sum_r e^{ikr} c_r, \quad d_k = \frac{1}{N} \sum_r e^{ikr} d_r,$$

(20)

be the Fourier transformed operators of the site annihilation operators $c_r$ and $d_r$ respectively. From Eq.(13) we get

$$c_{k\downarrow} = d_{k\dagger}, \quad c_{k\uparrow} = d_{-k\dagger}^\dagger, \quad Q = (\pi, \pi).$$

(21)

The ground state with the Fermi sea explicitly written is given by $|\Psi^{[0]}_{AF}\rangle = |\Phi^{[0]}_{AF}\rangle \otimes |\Sigma\rangle$ where $|\Sigma\rangle$ is the contribution from the filled shells:

$$|\Sigma\rangle = |\Sigma_\uparrow\rangle \otimes |\Sigma_\downarrow\rangle, \quad |\Sigma_\sigma\rangle = \prod_{c(k)<0} c_{k\sigma}^\dagger |0\rangle.$$ 

(22)

Modulo an overall phase factor, the particle-hole transformation yields

$$|\Sigma_\downarrow\rangle = \prod_{c(k)<0} c_{k\dagger}^\dagger |0\rangle = \prod_{c(k)<0} d_{k\dagger}^\dagger |0\rangle \equiv |\Sigma_\downarrow\rangle$$

(23)
Let $d_k$ be the operator obtained substituting $g_k$ with $d_k$, in the definition of $c_i$. We note that $\epsilon(k) < 0$ corresponds to $\epsilon(Q - k) > 0$. Then, the spin up filled shells state $|\Sigma_\uparrow \rangle$ can be written as

$$
|\Sigma_\uparrow \rangle = \prod_{\epsilon(k) < 0} d_k^\dagger |0\rangle = \prod_{\epsilon(k) < 0} d_{Q-k}^\dagger \prod_k d_k^\dagger |0\rangle.
$$

(24)

and hence

$$
|\Sigma_\uparrow \rangle \otimes |\Sigma_\downarrow \rangle = d_{N-1}^\dagger \ldots d_{N-1}^\dagger d_{2N-2}^\dagger \ldots d_{2N-2}^\dagger |\bar{\Sigma}_\uparrow \rangle \otimes |\bar{\Sigma}_\downarrow \rangle.
$$

(25)

The next step is to express $c_{\alpha \iota}$ in terms of $d_{\alpha \iota}$. By direct inspection one readily realizes that

$$
c_{\alpha \iota} = d_{\alpha \iota} \quad \forall i, \quad c_{\uparrow \uparrow} = \left\{ \begin{array}{ll}
d_{\uparrow \uparrow} & i = 1, \ldots, N - 1 \\
-d_{\uparrow \uparrow} & i = N, \ldots, 2N - 2
\end{array} \right.
$$

(27)

The above result implies that the raising operators $\hat{S}_{\alpha \iota}^\dagger$ in the $d$ picture are given by

$$
\hat{S}_{\alpha \iota}^\dagger = \left\{ \begin{array}{ll}
d_{\alpha \iota} d_{\alpha \iota}^\dagger & i = 1, \ldots, N - 1 \\
-d_{\alpha \iota} d_{\alpha \iota}^\dagger & i = N, \ldots, 2N - 2
\end{array} \right.
$$

(28)

These last three equations allow to rewrite the whole ground state $|\Psi_{AF}^{(0)}\rangle = |\Phi_{AF}^{(0)}\rangle \otimes |\Sigma\rangle$ in the new picture:

$$
|\Psi_{AF}^{(0)}\rangle = \frac{1}{\sqrt{N}} \left\{ \sum_{k = N/2}^{N-1} g_k \sum_{\tau_1 \ldots \tau_2} D_{\tau_1} \ldots D_{\tau_2} \sum_{j_1 \ldots j_{2N-2}} D_{j_1} \ldots D_{j_{2N-2}} \right. \\
\times d_{1,\tau_1} \ldots d_{N-1,\tau_1} d_{2N-2,\tau_2} \ldots d_{2N-2,\tau_2} |\bar{\Sigma}_\uparrow \rangle \otimes |\bar{\Sigma}_\downarrow \rangle + \\
+ \frac{1}{\sqrt{N}} \left\{ \sum_{k = N/2}^{N-1} g_k \sum_{\tau_1 \ldots \tau_2} D_{\tau_1} \ldots D_{\tau_2} \sum_{j_1 \ldots j_{2N-2}} D_{j_1} \ldots D_{j_{2N-2}} \right. \\
\times d_{1,\tau_1} \ldots d_{N-1,\tau_1} d_{2N-2,\tau_2} \ldots d_{2N-2,\tau_2} |\bar{\Sigma}_\uparrow \rangle \otimes |\bar{\Sigma}_\downarrow \rangle = \\
= \frac{1}{\sqrt{N}} \left\{ \sum_{k = N/2}^{N-1} g_k \sum_{\tau_1 \ldots \tau_2} \sum_{j_1 \ldots j_{2N-2}} D_{\tau_1} \ldots D_{\tau_2} D_{j_1} \ldots D_{j_{2N-2}} \right. \\
\times d_{1,\tau_1} \ldots d_{N-1,\tau_1} d_{2N-2,\tau_2} \ldots d_{2N-2,\tau_2} |\bar{\Sigma}_\uparrow \rangle \otimes |\bar{\Sigma}_\downarrow \rangle + \\
+ \frac{1}{\sqrt{N}} \left\{ \sum_{k = N/2}^{N-1} g_k \sum_{\tau_1 \ldots \tau_2} \sum_{j_1 \ldots j_{2N-2}} D_{\tau_1} \ldots D_{\tau_2} D_{j_1} \ldots D_{j_{2N-2}} \right. \\
\times d_{1,\tau_1} \ldots d_{N-1,\tau_1} d_{2N-2,\tau_2} \ldots d_{2N-2,\tau_2} |\bar{\Sigma}_\uparrow \rangle \otimes |\bar{\Sigma}_\downarrow \rangle.
$$

(29)

Therefore, the singlet ground state has the following form

$$
|\Psi_{AF}^{(0)}\rangle = \sum_{\Gamma} u_{\Gamma} D_{\tau_1}^\dagger |\bar{\Sigma}_\uparrow \rangle \otimes D_{\tau_2}^\dagger |\bar{\Sigma}_\downarrow \rangle,
$$

(30)

where $\Gamma = \{ \gamma_1, \ldots, \gamma_{N-1} \}$ with $1 \leq \gamma_1 < \ldots < \gamma_{N-1} \leq 2N - 2$ and $D_{\Gamma}^\dagger = d_{\gamma_1}^\dagger \ldots d_{\gamma_{N-1}}^\dagger$. $u_{\Gamma}$ is the amplitude corresponding to the configuration $\Gamma$. If in $\Gamma$ there are $p$ indices between 1 and $N - 1$ and $N - 1 - p$ indices between $N$ and $2N - 2$, or vice versa, the amplitude $u_{\Gamma}$ is given by

$$
u_{\Gamma} = \frac{1}{\sqrt{N}} 2^{N/2 - p}.
$$

(31)

We conclude that the Lieb matrix is already diagonal in the local basis, and the nonvanishing diagonal elements are $u_{\Gamma} > 0$. Thus it is positive semidefinite, which is consistent with its use as the ground state. We are now in position to calculate the correlation functions.
IV. THE SPIN CORRELATION FUNCTION

In this Section we will explicitly write down an exact analytic formula for the spin correlation function of the half filled Hubbard model in the limit of vanishing interaction. In particular we evaluate

\[ G_{\text{spin}}(r) = \langle \Psi_{AP}^{[0]} | S_r \cdot S_0 | \Psi_{AP}^{[0]} \rangle, \quad S_0 \equiv S_{r=(0,0)} \]  

where \( S_r = (\hat{S}_r^x, \hat{S}_r^y, \hat{S}_r^z) \) is the spin vector operator at site \( r \) with components

\[ \hat{S}_r^x = \frac{1}{2}(\hat{S}_r^+ + \hat{S}_r^-), \quad \hat{S}_r^y = \frac{1}{2i}(\hat{S}_r^+ - \hat{S}_r^-), \quad \hat{S}_r^z = \frac{1}{2}(\hat{n}_{r\uparrow} - \hat{n}_{r\downarrow}) \]  

and

\[ \hat{S}_r^+ = c_{r\uparrow} \hat{c}_{r\downarrow}, \quad \hat{S}_r^- = (\hat{S}_r^+)^\dagger = c_{r\downarrow}^\dagger \hat{c}_{r\uparrow}. \]  

Taking into account that \( \Psi_{AP}^{[0]} \) is a singlet, one has \( \langle \hat{S}_r^x \hat{S}_0^x \rangle = \langle \hat{S}_r^y \hat{S}_0^y \rangle = \langle \hat{S}_r^z \hat{S}_0^z \rangle \) and hence

\[ G_{\text{spin}}(r) = \frac{3}{4} [\langle \hat{S}_r^- \hat{S}_0^+ + \hat{S}_r^+ \hat{S}_0^- \rangle] \]  

with \( \hat{S}_r^\pm = \hat{S}_r^\pm r_{-r,(0,0)} \) and \( (\ldots) \) means the expectation value over the ground state \( |\Psi_{AP}^{[0]}\rangle \). Since \( |\Psi_{AP}^{[0]}\rangle \) is a real linear combination of real basis vectors, \( G^{-+}(r) = \langle \hat{S}_r^- \hat{S}_0^+ \rangle \in \mathbb{R} \) \( \forall r \) and this implies

\[ G^{-+}(r) = G^{-+}(r)^* = \langle \hat{S}_r^- \hat{S}_0^+ \rangle = \langle \hat{S}_r^+ \hat{S}_0^- \rangle - 2\Delta_{r,0} \langle \hat{S}_r^z \rangle. \]  

Noting that \( |\Psi_{AP}^{[0]}\rangle \) is a translation invariant state, \( \langle \hat{S}_0^\pm \rangle = \frac{1}{N} \sum_r \langle \hat{S}_r^\pm \rangle = \frac{1}{N} \langle \hat{S}^\pm \rangle = 0 \) and hence

\[ G^{-+}(r) = \langle \hat{S}_r^+ \hat{S}_0^- \rangle = G^{+-}(r). \]  

This last equation allow us to express the spin correlation function \( G_{\text{spin}}(r) \) in terms of \( G^{+-}(r) \) only

\[ G_{\text{spin}}(r) = \frac{3}{2} G^{+-}(r), \]  

and the original problem is reduced to the calculation of \( G^{+-}(r) \). In the following we will show that \( G^{+-}(r) \) can be expressed in terms of three main contributions, two of which easily computable in the particle-hole transformed picture. Therefore, it is convenient to express \( G^{+-}(r) \) in terms of the \( d \)'s operators:

\[ G^{+-}(r) = \langle \Gamma_1 | d_{\Gamma_1}^\dagger d_{\Gamma_2}^\dagger | \Gamma_2 \rangle = (-)^{x+y} \sum_{\Gamma_1, \Gamma_2} \langle \Gamma_1 | d_{\Gamma_1}^\dagger d_{\Gamma_2}^\dagger | \Gamma_2 \rangle \times \]  

\[ \times \langle \Sigma_1 | D_{\Gamma_1} d_{\Gamma_2}^\dagger | \Sigma_2 \rangle \equiv \langle \Gamma_1 | D_{\Gamma_1} G_{\Gamma_1,\Gamma_2}(r) | \Gamma_2 \rangle^2, \]  

where, dropping the spin index,

\[ G_{\Gamma_1,\Gamma_2}(r) = \langle \Gamma_1 | d_{\Gamma_2}^\dagger G_{\Gamma_2}^\dagger | \Gamma_2 \rangle, \quad |\Gamma\rangle = D_{\Gamma}^\dagger |\Sigma\rangle. \]  

Here and in the following \( c_{00} \equiv c_{r=(0,0)} \) and \( d_{00} \equiv d_{r=(0,0)} \). Since the \( w \)'s are non-negative, Eq.(39) shows that \( G^{+-}(r) \) is positive if \( r \) belongs to the sublattice \( A \) containing \( r = (0,0) \) and negative otherwise. This was pointed out in Ref. [17]. All the information on the spin correlation function is enclosed into the site-dependent matrix elements \( G_{\Gamma_1,\Gamma_2}(r) \). To evaluate them we write the annihilation operator \( d \) as the sum of three pieces

\[ d_r = \frac{1}{N} \sum_k e^{i k \cdot r} d_k = \frac{\sqrt{|S_h|}}{N} d_1(r) + \frac{\sqrt{|S|}}{N} d_2(r) + \frac{\sqrt{|S|}}{N} d_3(r) \equiv \rho_{h1} d_1(r) + \rho d_2(r) + \rho d_3(r), \]  

with

\[ d_1(r) = \frac{1}{\sqrt{|S|}} \sum_{\langle k \rangle = 0} e^{i k \cdot r} d_k, \quad d_2(r) = \frac{1}{\sqrt{|S|}} \sum_{\langle k \rangle < 0} e^{i k \cdot r} d_k, \quad d_3(r) = \frac{1}{\sqrt{|S|}} \sum_{\langle k \rangle > 0} e^{i k \cdot r} d_k \]  

where
and $|S_{n}| = 2N - 2$, $|S| = \frac{1}{2}(N^2 - |S_{n}|)$. We observe that $d_1(0) = d_1(r = (0, 0))$ belongs to $A_f$, and that it can be written as a real linear combination of all the $A_f$-symmetric local annihilation operators of the local basis. By a unitary transformation on this $A_f$-subspace we may arrange that $d_1(0)$ is the new $d_1$. Thus, from now on, the one-body local basis $\{d^i_1(0), i = 1, \ldots, 2N - 2\}$, is such that the set of the $A_f$-symmetric local states contains $d_1^z(0)|0\rangle$ and $d_1^z(0)|0\rangle$.

Taking Eq.(41) into account one can express $G_{12}(r)$ as the sum of two terms:

$$G_{12}(r) = \rho_{hf}(\Pi_1) d_1(r) d_1(\Pi_2) + \rho_{hf}(\Pi_1) d_2(r) d_2(\Pi_2) \equiv \rho_{hf}^2 G_{12}^{[hf]}(r) + \rho_{hf}^2 G_{12}^{[f]}(r),$$

with $d_1 \equiv d_1(0)$ and $d_2 \equiv d_2(0) \equiv d_2(r = (0, 0))$. $G_{12}^{[f]}(r)$ can be easily evaluated:

$$G_{12}^{[f]}(r) = (\Pi_1) d_1^f(r) d_2(\Pi_2) = \delta_{\Pi_1} \sum_{\epsilon(k_1) < 0} \sum_{\epsilon(k_2) < 0} e^{-i k_1 \cdot r} \frac{1}{|S|} \langle \Sigma | d^f_{k_1} d_{k_2} | \Sigma \rangle = \delta_{\Pi_1} \frac{T(r)}{|S|}$$

where $T(r) = \sum_{\epsilon(k) < 0} e^{-i k \cdot r}$ is the trace of the translation matrix in the Hilbert space spanned by the negative energies one-body plane-wave states. Taking into account Eqs.(43),(44), $G^{-+}(r)$ in Eq.(39) can be rewritten as

$$G^{-+}(r) = (-)^{x+y} \sum_{\Pi_1 \Pi_2} \sum_{\Pi_1} w_{\Pi_1} w_{\Pi_2} G_{12}^{[hf]}(r) + 2 \rho_{hf}^2 \sum_{\Pi_1} \sum_{\Pi_2} T(r) w_{\Pi_1}^2 G_{12}^{[hf]}(r) + \rho_{hf}^4 \frac{T(r)^2}{|S|^2} \sum_{\Pi_1} w_{\Pi_1}^2 \delta_{\Pi_1, \Pi_2}.$$  

By definition $\sum_{\Pi_1} w_{\Pi_1}^2 = \langle \Psi_0 | \psi_{HF} \rangle \langle \psi_{HF} | \Psi_0 \rangle = 1$. To evaluate the diagonal matrix elements $G_{11}^{[hf]}(r)$ we need to use the antiferromagnetic property. In the local basis, the one-body translation matrix has an antidiagonal block form if $x + y$ is odd and hence a diagonal block form otherwise. Therefore $d_1(r)$ can be expanded as

$$d_1(r) = \begin{cases} \sum_{i=1}^{N-1} t_i(r) d_i, & t_i(r) \in \mathbb{R} \quad x + y \text{ even} \\ \sum_{i=1}^{2N-2} t_i(r) d_i, & t_i(r) \in \mathbb{R} \quad x + y \text{ odd} \end{cases}$$

and $G_{11}^{[hf]}(r)$ becomes

$$G_{11}^{[hf]}(r) = (\Pi_1) d_1^f(r) d_1(\Pi_2) = \begin{cases} t_1(r) \delta_{\Pi_1, \Pi_1} & x + y \text{ even} \\ 0 & x + y \text{ odd} \end{cases}$$

where $\gamma_1$ is the first index of the configuration $\Pi$ (we remind that $\Pi = \{\gamma_1, \ldots, \gamma_{N-1}\}$ with $1 \leq \gamma_1 < \ldots < \gamma_{N-1} \leq 2N - 2$). Substituting this result into Eq.(45) we see we need to evaluate $\sum_{\Pi_1} w_{\Pi_1}^2 \delta_{\Pi_1, \Pi_2}$. This can be done by observing that $|\Phi_{0}^{[hf]}\rangle$ can be rewritten in the $c$ picture as

$$|\Phi_{0}^{[hf]}\rangle = |\Phi_{0}^{[hf]}\rangle^{+} - |\Phi_{0}^{[hf]}\rangle^{0}$$

with

$$|\Phi_{0}^{[hf]}\rangle^{+} = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-2} \sum_{i_k > \ldots > i_1 = 2} \cdots \sum_{j_k > \ldots > j_1 = N} S_{i_k}^{+} \cdots S_{i_1}^{+} S_{j_k}^{-} \cdots S_{j_1}^{-} c_{1}^{\uparrow} \cdots c_{N-1}^{\uparrow} c_{N}^{\uparrow} \cdots c_{2N-2}^{\uparrow} |0\rangle$$

$$|\Phi_{0}^{[hf]}\rangle^{0} = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-2} \sum_{i_k > \ldots > i_1 = 2} \cdots \sum_{j_k > \ldots > j_1 = N} S_{i_k}^{+} \cdots S_{i_1}^{+} S_{j_k}^{-} \cdots S_{j_1}^{-} c_{1}^{\uparrow} \cdots c_{N-1}^{\uparrow} c_{N}^{\uparrow} \cdots c_{2N-2}^{\uparrow} |0\rangle$$

and

$$f_k = \begin{cases} g_{N/2-k} & k = 0, \ldots, N/2 - 1 \\ g_{k+1-N/2} & k = N/2, \ldots, N - 1 \end{cases}$$

All the configurations contained in $|\Phi_{0}^{[hf]}\rangle^{+}$ are such that in the particle-hole transformed picture $\delta_{\gamma_1} = 1$. On the other hand, all the configurations contained in $|\Phi_{0}^{[hf]}\rangle^{0}$ are such that in the particle-hole transformed picture $\delta_{\gamma_1} = 0$. Therefore

$$\sum_{\Pi_1} w_{\Pi_1}^2 \delta_{\Pi_1, \Pi_2} = \langle \Phi_{0}^{[hf]} | \Phi_{0}^{[hf]}^{+} \rangle = \langle \Phi_{0}^{[hf]} | \Phi_{0}^{[hf]}^{0} \rangle = \frac{1}{2}.$$
The second term in Eq.(45) is totally determined once we know \( t_1(\mathbf{r}) \). By definition

\[
t_1(\mathbf{r}) = \langle 0 | d_1^\dagger(\mathbf{r}) d_1(0) \rangle = \mathcal{T}_{hf}(\mathbf{r}) |\mathcal{S}_{hf}\rangle,
\]

where \( \mathcal{T}_{hf}(\mathbf{r}) = \sum_{\epsilon(\mathbf{k})=0} e^{i\mathbf{k}\cdot\mathbf{r}} \) is the trace of the translation matrix in the Hilbert space spanned by the \( \epsilon(\mathbf{k}) = 0 \) one-body plane-wave states. In the last equality of Eq.(53) we have used Eq.(42). By noting that \( \mathcal{T}_{hf}(\mathbf{r}) \) vanishes any time \( x + y \) is odd, one obtains for \( G^{-\pm}(\mathbf{r}) \) the following result

\[
G^{-\pm}(\mathbf{r}) = (-)^{x+y} \{ \rho_{hf}^2 \sum_{\Gamma_1 \Gamma_2} w_{\Gamma_1} w_{\Gamma_2} G^{[hf]}_{\Gamma_1 \Gamma_2}(\mathbf{r})^2 + \frac{1}{N^2} \mathcal{T}(\mathbf{r}) [ \mathcal{T}(\mathbf{r}) + \mathcal{T}_{hf}(\mathbf{r}) ] \}
\]

where we have used Eqs.(47),(52),(53).

In order to make this result more explicit, we perform the sum in the first term of Eq.(54). It can be easily calculated coming back to the original c picture. Indeed

\[
(-)^{x+y} \sum_{\Gamma_1 \Gamma_2} w_{\Gamma_1} w_{\Gamma_2} G^{[hf]}_{\Gamma_1 \Gamma_2}(\mathbf{r})^2 = \langle \Psi^{[hf]}_{A_F}|c^\dagger_{1,\uparrow}c^\dagger_{1,\downarrow}\mathcal{T}(\mathbf{r})c_{1,\downarrow}c_{1,\uparrow}|\Psi^{[hf]}_{A_F}\rangle = \langle \Phi^{[0]}_\downarrow|c^\dagger_{1,\downarrow}c_{1,\uparrow}\tilde{T}(\mathbf{r})c^\dagger_{1,\uparrow}c_{1,\downarrow}|\Phi^{[0]}_\downarrow\rangle \equiv X(\mathbf{r})
\]

where \( |\Phi^{[0]}_\downarrow\rangle \) is defined in Eq.(50) and \( \tilde{T}(\mathbf{r}) \) is the translation operator by \( \mathbf{r} \): \( \tilde{T}(\mathbf{r})c_1(\mathbf{r}) = c_1(\mathbf{r}+\mathbf{r}) \). As usual \( c_i \) is given by the same expression which defines \( d_i \), with \( d_k \rightarrow c_k \). Therefore, according to the new expression of \( d_1 = d_1(0) \), we have \( c_1 = \frac{1}{|\mathcal{T}_{hf}|} \sum_{\epsilon(\mathbf{k})=0} c_k \) and this is why \( c_1 = c_1(0) = c_1(\mathbf{r} = (0,0)) \) shows up in Eq.(55). Finally we observe that the spin-dependent filled Fermi sea \( |\Sigma_a\rangle \) can contribute only a phase factor corresponding to its momentum; since \( |\Sigma_a\rangle \) has vanishing momentum the phase factor is exactly 1.

The explicit evaluation of \( X(\mathbf{r}) \) is deferred to Appendix A. Here we report the final result

\[
X(\mathbf{r}) = \frac{(-)^{x+y}}{|\mathcal{T}_{hf}|^2} \left\{ \begin{array}{ll}
A + B \times \mathcal{T}_{hf}(\mathbf{r}) & x + y \text{ even} \\
A + B \times (4N - 4) & x + y \text{ odd}
\end{array} \right.
\]

where \( A \) and \( B \) are two \( N \)-dependent constants. Eventually, substituting this last result in Eq.(54) and taking into account Eq.(38), we get the full analytic expression of the spin correlation function

\[
G_{\text{spin}}(\mathbf{r}) = \frac{1}{2} \frac{(-)^{x+y}}{N^2} \left\{ \mathcal{T}(\mathbf{r})[\mathcal{T}(\mathbf{r}) + \mathcal{T}_{hf}(\mathbf{r})] + \left\{ \begin{array}{ll}
A + B \times \mathcal{T}_{hf}(\mathbf{r}) & x + y \text{ even} \\
A + B \times (4N - 4) & x + y \text{ odd}
\end{array} \right. \right\}
\]

In this form it is not hard to show that independent of the numerical value of the two constants \( A \) and \( B \) the sum rule

\[
\sum_{\mathbf{r}} G_{\text{spin}}(\mathbf{r}) = 0
\]

holds. Indeed, let us consider the identities

\[
\sum_{\mathbf{r}} (-1)^{x+y} \mathcal{T}(\mathbf{r})^2 = \sum_{\mathbf{r}} \sum_{\epsilon(\mathbf{k}),\epsilon(\mathbf{k}')<0} (-1)^{x+y} e^{-i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{r}} = \sum_{\mathbf{r}} \sum_{\epsilon(\mathbf{k}),\epsilon(\mathbf{k}')<0} e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{Q})\cdot\mathbf{r}};
\]

since the \( \mathbf{r} \) summation yields \( N^2 \) times a \( \delta \) function, and the \( \delta \) function is never satisfied (if \( \epsilon(\mathbf{k}) < 0 \) then \( \epsilon(\mathbf{Q} - \mathbf{k}) > 0 \)), one finds that

\[
\sum_{\mathbf{r}} (-1)^{x+y} \mathcal{T}(\mathbf{r})^2 = 0,
\]

and, similarly

\[
\sum_{\mathbf{r}} (-1)^{x+y} \mathcal{T}(\mathbf{r}) \mathcal{T}_{hf}(\mathbf{r}) = 0.
\]

On the other hand, since

\[
\sum_{\mathbf{r} \in \mathcal{A}} e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{N^2}{2} (\delta_{\mathbf{k},0} + \delta_{\mathbf{k},\mathbf{Q}}),
\]

where \( \mathcal{A} \) is the sublattice with sites having \( x + y \) even, one gets

\[
\sum_{\mathbf{r} \in \mathcal{A}} \mathcal{T}_{hf}(\mathbf{r})^2 = \frac{N^2}{2} (4N - 4)
\]

and hence Eq.(58).
V. THE CHARGE CORRELATION FUNCTION

The charge and spin correlation functions are closely related. Let $\hat{n}_r^{[\pm]} = \hat{n}_{r\uparrow} \pm \hat{n}_{r\downarrow}$; so, $\hat{n}_r^{[\pm]}$ is the number operator, while $\hat{n}_r^{[\pm]}$ is twice the $z$ component of the spin on the site $r$. Then, the charge correlation function is given by

$$G_{\text{charge}}(r) \equiv \langle \Psi_{AF}^{[0]} | \hat{n}_r^{[\pm]} \hat{n}_0^{[\pm]} | \Psi_{AF}^{[0]} \rangle,$$

while the spin correlation function can be written as

$$G_{\text{spin}}(r) = 3 \langle \Psi_{AF}^{[0]} | \hat{S}_x^r \hat{S}_z^0 | \Psi_{AF}^{[0]} \rangle = \frac{3}{4} \langle \Psi_{AF}^{[0]} | \hat{n}_r^{[-]} \hat{n}_0^{[-]} | \Psi_{AF}^{[0]} \rangle,$$

where $\hat{n}_0^{[\pm]} \equiv \hat{n}_{r=(0,0)}$. Let

$$| \Psi_{AF}^{[0]} \rangle = | \Psi_{\uparrow}^{[0]} \rangle - | \Psi_{\downarrow}^{[0]} \rangle,$$

with $| \Psi_{\sigma}^{[0]} \rangle = | \Phi_{\sigma}^{[0]} \rangle \otimes | \Sigma \rangle$, be a suitable decomposition of the singlet ground state wave function, see Eq.(48). Exploiting the invariance of $| \Psi_{\sigma}^{[0]} \rangle$ for simultaneous flips of $\sigma$ and $\sigma'$, we get

$$G_{\text{charge}}(r) = 2 \langle \Psi_{\uparrow}^{[0]} | \hat{n}_r^{[\pm]} \hat{T}^r(r) \hat{n}_0^{[\pm]} | \Psi_{\uparrow}^{[0]} \rangle - \langle \Psi_{\uparrow}^{[0]} | \hat{n}_r^{[\mp]} \hat{T}^r(r) \hat{n}_0^{[\pm]} | \Psi_{\uparrow}^{[0]} \rangle \rangle$$

$$G_{\text{spin}}(r) = \frac{3}{2} \left[ \langle \Psi_{\uparrow}^{[0]} | \hat{n}_r^{[-]} \hat{T}^r(r) \hat{n}_0^{[-]} | \Psi_{\uparrow}^{[0]} \rangle - \langle \Psi_{\uparrow}^{[0]} | \hat{n}_r^{[-]} \hat{T}^r(r) \hat{n}_0^{[-]} | \Psi_{\uparrow}^{[0]} \rangle \right],$$

where $\hat{T}(r)$ is the operator of the translation by $r$, such that

$$\hat{n}_{r\sigma} = \hat{T}^r(r) \hat{n}_{0\sigma} \hat{T}(r)^r$$

and $\hat{T}^r(r) | \Psi_{AF}^{[0]} \rangle = | \Psi_{AF}^{[0]} \rangle$ has been used. The action of $\hat{n}_r^{[\pm]}$ on the state $| \Psi_{\sigma}^{[0]} \rangle$ can be easily evaluated. We can express $c_r$ as the sum of three operators like in Eq.(41)

$$c_r = \rho_{h_f} c_1(r) + \rho c_\xi(r) + c_\xi(r)$$

where $c_1$, $c_\xi$ and $c_\xi$ are defined as $d_1$, $d_\xi$ and $d_\xi$ in Eq.(42), but $d_\xi$ must be substituted with $c_\xi$. Then we get

$$\hat{n}_0^{[\pm]} | \Psi_{\uparrow}^{[0]} \rangle = (\hat{n}_{0\uparrow} \pm \hat{n}_{0\downarrow}) | \Psi_{\uparrow}^{[0]} \rangle = \left( \rho_{h_f}^2 + \rho^2 \pm \rho^2 \right) P_{c_\xi c_\xi},$$

$$\hat{n}_0^{[\pm]} | \Psi_{\downarrow}^{[0]} \rangle = \left( \rho_{h_f}^2 + \rho^2 \pm \rho^2 \right) P_{c_\xi c_\xi},$$

(73)

Hence $(\hat{n}_{0\uparrow} \pm \hat{n}_{0\downarrow}) | \Psi_{\uparrow}^{[0]} \rangle$ can be expressed as a linear combination of five orthogonal states. By means of these two last equations one gets

$$\langle \Psi_{\uparrow}^{[0]} | \hat{n}_r^{[\pm]} \hat{T}^r(r) \hat{n}_0^{[\pm]} | \Psi_{\uparrow}^{[0]} \rangle = (\rho_{h_f}^2 + \rho^2 \pm \rho^2) \langle \Sigma | c_\xi c_\xi \hat{T}(r) c_\xi c_\xi \hat{T}(r) | \Sigma \rangle | \Phi_{\uparrow}^{[0]} \rangle | \Phi_{\uparrow}^{[0]} \rangle +$$

$\rho^2 P_{c_\xi c_\xi} \langle \Psi_{\uparrow}^{[0]} | c_1^r \hat{T}(r) c_1 \hat{T}(r)^r | \Phi_{\uparrow}^{[0]} \rangle | \Sigma | c_\xi c_\xi \hat{T}(r) c_\xi c_\xi \hat{T}(r)^r | \Sigma \rangle +$$

$\langle \Psi_{\uparrow}^{[0]} | c_1^r \hat{T}(r) c_1 \hat{T}(r)^r | \Phi_{\uparrow}^{[0]} \rangle | \Sigma | c_\xi c_\xi \hat{T}(r) c_\xi c_\xi \hat{T}(r)^r | \Sigma \rangle \rangle$

(74)

and

$$\langle \Psi_{\downarrow}^{[0]} | \hat{n}_r^{[\pm]} \hat{T}^r(r) \hat{n}_0^{[\pm]} | \Psi_{\downarrow}^{[0]} \rangle = (\rho_{h_f}^2 + \rho^2 \pm \rho^2) \langle \Sigma | c_\xi c_\xi \hat{T}(r) c_\xi c_\xi \hat{T}(r) | \Sigma \rangle | \Phi_{\downarrow}^{[0]} \rangle | \Phi_{\downarrow}^{[0]} \rangle +$$

$\rho^2 P_{c_\xi c_\xi} \langle \Psi_{\downarrow}^{[0]} | c_1^r \hat{T}(r) c_1 \hat{T}(r)^r | \Phi_{\downarrow}^{[0]} \rangle | \Sigma | c_\xi c_\xi \hat{T}(r) c_\xi c_\xi \hat{T}(r)^r | \Sigma \rangle \rangle$

since $| \Sigma | c_\xi c_\xi \hat{T}(r) c_\xi c_\xi \hat{T}(r)^r | \Sigma \rangle$ does not depend on $\sigma$. The number of scalar products can be further reduced: we recall that $| \Phi_{AF}^{[0]} \rangle \equiv | \Phi_{\uparrow}^{[0]} \rangle - | \Phi_{\downarrow}^{[0]} \rangle$ is an eigenstate of the total momentum with vanishing eigenvalue:

$$1 = \langle \Phi_{AF}^{[0]} | \hat{T}(r) | \Phi_{AF}^{[0]} \rangle = 2 \left[ \langle \Phi_{\uparrow}^{[0]} | \hat{T}(r) | \Phi_{\uparrow}^{[0]} \rangle - \langle \Phi_{\downarrow}^{[0]} | \hat{T}(r) | \Phi_{\downarrow}^{[0]} \rangle \right]$$

(76)
Substituting Eq.(76) into Eq.(74) and then subtracting Eq.(73) term by term yields

\[
\langle \Psi_0^0 | \hat{n}_0^{\pm} \hat{T}(r) \hat{n}_0^{\pm} | \Psi_0^0 \rangle - \langle \Psi_0^0 | \hat{n}_0^{\pm} \hat{T}(r) \hat{n}_0^{\pm} | \Psi_0^0 \rangle = \pm \frac{\rho_h^2}{2} + \rho^2 \pm \rho^2 + \rho^4 \langle \Sigma c_{\uparrow} c_{\uparrow} \hat{T}(r) c_{\downarrow} c_{\downarrow} | \Sigma \rangle + \\
+ \rho^2 \rho_h^2 \left[ \langle \Phi_0^0 | c_{\uparrow} \hat{T}(r) c_{\uparrow} | \Phi_0^0 \rangle \langle \Sigma | c_{\uparrow} \hat{T}(r) c_{\uparrow} | \Sigma \rangle + \langle \Phi_0^0 | c_{\downarrow} \hat{T}(r) c_{\downarrow} | \Phi_0^0 \rangle \langle \Sigma | c_{\downarrow} \hat{T}(r) c_{\downarrow} | \Sigma \rangle \right] + \\
+ \left[ (1 \pm (1)) (\rho_h^2 + \rho^2 \pm \rho^2)^2 \right] \langle \Phi_0^0 | \hat{T}(r) | \Phi_0^0 \rangle
\]

and so, since \( \rho_h^2 + 2 \rho^2 = 1 \),

\[
G_{\text{charge}}(r) = 1 + \frac{\rho}{2} G_{\text{spin}}(r) + \rho_h^2 \left[ 1 - 4 Y(r) \right],
\]

where

\[
Y(r) \equiv \langle \Phi_0^0 | \hat{T}(r) | \Phi_0^0 \rangle.
\]

We postpone to Appendix B the explicit calculation of \( Y(r) \). Here we limit to present the final results

\[
Y(r) = \frac{1}{2} + \frac{(x+y)^2}{2 \rho_h t} \times \left\{ \begin{array}{ll}
D + E \times T_h(r)^2 & x + y \text{ even} \\
D + E \times (4N - 4) & x + y \text{ odd}
\end{array} \right.
\]

As for the spin correlation function one can easily verify that independent of the numerical value of the two \( N \)-constants \( D \) and \( E \), the sum rule

\[
\sum_r G_{\text{charge}}(r) = N^2
\]

is satisfied.

VI. RESULTS AND DISCUSSION

Most of the available data on the half filled Hubbard Model on a square lattice refer to the 4 \( \times \) 4 cluster, see for example Ref. [5]. In the left hand side of Figure 1 we report a classical representation of the spin correlations in the 4 \( \times \) 4 lattice: the length of the lines is proportional to the absolute value of the correlation function, and the sign is positive for the lines going up. This representation was adopted in Ref. [5] and our result is identical to that reported there, which was obtained by second-order perturbation theory on the computer.

![Graph showing spin correlation function](image-url)
More data [18] [19] on the $4 \times 4$ cluster were obtained by Fano, Ortolani and Parola by exact diagonalisation augmented by an intensive use of Group theory techniques. In the right hand side of Figure 1 we report the spin correlation function in real space, $G_{\text{spin}}(r)$ in Eq.(57), along a triangular path. Although our results are exact for $U \to 0$, remarkably the trend is quite the same as the one reported in Ref. [18] for $U = 4$. An overall factor of 4 depends from the definition of the spin operators in [18], lacking the usual 1/2 factor.

The analytic expression of the spin correlation function in Eq.(57) agree with the important Shen-Qiu-Tian [17] theorem, which has been extended to finite temperatures quite recently [20]. This theorem states that the spin correlation function must be positive on one sublattice and negative on the other. This applies to the results for the $4 \times 4$, $6 \times 6$, $8 \times 8$ and $10 \times 10$ clusters as well, as shown in Figure 2. Essentially, the Shen-Qiu-Tian property is a consequence of the positive semidefinite ground state Lieb matrix, and we have explicitly verified this property in Section III above.

![Diagram](attachment:figure2.png)

**FIG. 2.** The spin correlation function in real space for the $4 \times 4$, $6 \times 6$, $8 \times 8$ and $10 \times 10$ clusters. The Shen-Qiu-Tian property is evident.

The Fourier transform of the spin correlation function

$$G_{\text{spin}}(k) \equiv \sum_{r} e^{ik \cdot r} G_{\text{spin}}(r)$$

is shown in Figure 3; the ticks on the $x$ axis correspond to the points $\Gamma \equiv (0, 0)$, $P \equiv (\pi, 0)$, $Q \equiv (\pi, \pi)$ and $\Gamma$ again, in $k$-space. The trend is seen to converge rather quickly to a characteristic shape which is strongly peaked in the $Q$ direction.
FIG. 3. The Fourier transform of the spin correlation functions in clusters of various sizes. The ticks of the x axis correspond to the Γ, P, Q and Γ, as usual.

The charge correlation function in real space shows characteristic structures with two intersecting channels at 45 degrees from the axes as exemplified in Figure 4 for the 10×10 case; at the intersection the correlation function presents a narrow hole. Similar trends are observed for the other clusters, although the intensity of the corrugation declines with increasing cluster size.

FIG. 4. Real space representation of the charge correlation function in the 4×4, 6×6, 8×8 and 10×10 clusters.

The Fourier transformed charge correlation function is dominated by a delta function at Γ ≡ (0, 0) resulting from the almost constant distribution in real space. In Figure 5 we have removed that delta. The figure
represents $G_{\text{charge}}(k) \equiv \sum_r e^{i k \cdot r} G_{\text{charge}}(r)$ along the path $\Gamma$, $P$, $Q$ and $\Gamma$ (see figure caption for details) for the 10 x 10 square lattice. Already at this cluster size $G_{\text{charge}}(k)$ shows a very similar trend to its asymptotic ($N \to \infty$) shape.

In conclusion, we have obtained explicit analytic expressions for the spin and charge correlation functions using a weak-coupling ground state wave function $|\Psi_{0,hf}^0\rangle$ of the half filled Hubbard Model on a square lattice. We compared our analytic results with the numerical data available in the literature. They always agree well; remarkably, provided that $U \leq t/N^2$, our predictions are good approximations to the exact diagonalization results.

As far as the non half-filled system is concerned, the same local formalism can be used to calculate the correlation functions of the doped Hubbard antiferromagnet, but first-order perturbation theory is not enough to single out a unique ground state. However, in the half filled ground state there are $2N - 2$ particles in the $\epsilon = 0$ shell that do not have double occupation; therefore, doping the system with two holes, one obtains a first-order ground state provided that a pair is annihilated belonging to the shell $S_h$; this must be a $W = 0$ pair. Since there are $W = 0$ pairs belonging to different irreps of the Space Group, the many-body ground state which is formed by annihilating the pair also has components of different symmetries. For each symmetry, we shall have different correlation functions to compute. Actually, we need second-order perturbation theory to resolve the degeneracy. This was done in Ref. [21] in the special case $N = 4$. On the other hand, the problem becomes trivial when the shell at the Fermi surface is totally filled since the non-interacting ground state is unique.

As pointed out in Ref. [22], one can use standard perturbation theory to calculate the correlation functions order by order in $U$; in the thermodynamic limit they can be expanded as an asymptotic series.

APPENDIX A: EVALUATION OF $X$

To evaluate $X(r) = (\Phi_{\uparrow}^0|^c_{1,\downarrow} c_{1,\uparrow} T(r) c_{1,\downarrow}^\dagger |\Phi_{\uparrow}^0\rangle)$ we need to consider separately the cases of even and odd $x + y$. In the first case, let $T(r)$ be the block-diagonal translation matrix in the local basis:

$$
\hat{T}(r)c_i^\dagger |0\rangle = \sum_{\gamma=1}^{2N-2} T(r)_{i,\gamma} c_\gamma^\dagger |0\rangle = \begin{cases} 
\sum_{a=1}^{N-1} T(r)_{i,a} c_a^\dagger |0\rangle, & i = 1, \ldots, N - 1 \\
\sum_{b=N}^{2N-2} T(r)_{i,b} c_b^\dagger |0\rangle, & i = N, \ldots, 2N - 2
\end{cases}.
$$

(A1)

We have

$$
\hat{T}(r)c_i^\dagger c_j^\dagger |\Phi_{\uparrow}^0\rangle = \frac{1}{\sqrt{N}} \sum_{a_1=1}^{N-1} \sum_{a_{N-1}=1}^{2N-2} \prod_{a=1}^{N-1} T(r)_{a,a} \prod_{b=N}^{2N-2} T(r)_{b,b} \times 
\sum_{k=0}^{N-2} (-)^k f_k \sum_{i_k > \ldots > i_1 = 2} \sum_{j_k > \ldots > j_1 = 1} \hat{S}_{a_1}^{i_1} \hat{S}_{a_1}^{i_1} \hat{S}_{a_1}^{j_1} \hat{S}_{a_1}^{j_1} \ldots \hat{S}_{a_1}^{j_1} \hat{S}_{a_1}^{j_1} \hat{c}_{a_1}^\dagger \hat{c}_{a_1}^\dagger \hat{c}_{a_1}^\dagger \ldots \hat{c}_{a_1}^\dagger \hat{c}_{a_1}^\dagger |0\rangle
$$

(A2)

and hence

FIG. 5. The Fourier transform of the charge correlation function in the 10 x 10 cluster; a delta function at the $\Gamma$ point is removed. The ticks of the $x$ axis correspond to the $\Gamma$, $P$, $Q$ and $\Gamma$, as usual.
\[
X(\mathbf{r}) = \frac{1}{N} \sum_{\alpha_1 \cdots \alpha_{N-1}=1}^{N-1} \sum_{\beta_1 \cdots \beta_{N-1}=N}^{2N-2} \prod_{a=1}^{N-1} T(\mathbf{r})_{a, \alpha_a} \prod_{b=N}^{2N-2} T(\mathbf{r})_{b, \beta_b} \sum_{k=0}^{N-2} \frac{f_k^2}{k!} \times \\
\times \left\{ \sum_{m_k \cdots m_1=2}^{N-1} \sum_{i_k \cdots i_1=1}^{N-1} (0|c_{N-1, \cdots, c_{1, \cdots, c_{N-1}, \cdots, c_1}|0) \right\} \times \\
\times \left\{ \sum_{n_k \cdots n_1=N}^{2N-2} \sum_{j_k \cdots j_1=1}^{N-1} (0|c_{2N-2, \cdots, c_{N, \cdots, c_{2N-2}, \cdots, c_1}|0) \right\} \right\} 
\]

(A3)

Taking into account that the annihilation operators in the second and third row of the above equation are all different (in particular their indices are \(1, \ldots, N-1\) in the second row and \(N, \ldots, 2N-2\) in the third row), a great simplification takes place:

\[
\sum_{i_k \cdots i_1=2}^{N-1} S_{\alpha_1} \cdots S_{\alpha_{N-1}} \varepsilon c_{\alpha_1, \cdots, \alpha_{N-1}} |0 = \varepsilon c_{\alpha_1, \cdots, \alpha_{N-1}} \sum_{i_k \cdots i_1=1, \neq \alpha_1} (0|c_{N-1, \cdots, c_{1, \cdots, c_{N-1}, \cdots, c_1}|0) + \ldots 
\]

(A4)

\[
\sum_{j_k \cdots j_1=1}^{N-1} \tilde{S}_{\beta_1} \cdots \tilde{S}_{\beta_{N-1}} \varepsilon c_{\beta_1, \cdots, \beta_{N-1}} |0 = \tilde{\varepsilon} c_{\beta_1, \cdots, \beta_{N-1}} \sum_{j_k \cdots j_1=N}^{2N-2} (0|c_{2N-2, \cdots, c_{N, \cdots, c_{2N-2}, \cdots, c_1}|0) + \ldots 
\]

(A5)

where \(\varepsilon\) is the totally antisymmetric tensor with \(N-1\) indices, while \(\tilde{\varepsilon} c_{\beta_1, \cdots, \beta_{N-1}} \equiv \varepsilon c_{\beta_1, \cdots, \beta_{N-1}, \cdots, N+1}\) and the dots mean that we are neglecting other terms whose contribution to the scalar product is zero. On the right hand side of Eq.(A4) the summation indices \(i_k \cdots i_1\) run in the interval \(\{1, \ldots, N-1\}\) in such a way that none of them is equal to \(\alpha_1\). Using Eq.(A4), the second row of Eq.(A3) yields

\[
\varepsilon c_{\alpha_1, \cdots, \alpha_{N-1}} \sum_{m_k \cdots m_1=2}^{N-1} \sum_{i_k \cdots i_1=1, \neq \alpha_1} (0|c_{N-1, \cdots, c_{1, \cdots, c_{N-1}, \cdots, c_1}|0) = \\
= \varepsilon c_{\alpha_1, \cdots, \alpha_{N-1}} \left[ \delta_{\alpha_1} \left( \begin{array}{c} N-2 \\ k \end{array} \right) + (1 - \delta_{\alpha_1}) \left( \begin{array}{c} N-3 \\ k-1 \end{array} \right) \right] 
\]

(A6)

while using Eq.(A5), the third row of Eq.(A3) yields

\[
\tilde{\varepsilon} c_{\beta_1, \cdots, \beta_{N-1}} \sum_{n_k \cdots n_1=N}^{2N-2} \sum_{j_k \cdots j_1=N}^{N-1} (0|c_{2N-2, \cdots, c_{N, \cdots, c_{2N-2}, \cdots, c_1}|0) = \\
= \tilde{\varepsilon} c_{\beta_1, \cdots, \beta_{N-1}} \left( \begin{array}{c} N-1 \\ k \end{array} \right) . 
\]

(A7)

These two last results allow to rewrite \(X(\mathbf{r})\) as

\[
X(\mathbf{r}) = \frac{A}{|S_{h_f}|^2} + BC_{1,1}(r)T(\mathbf{r})_{1,1} 
\]

(A8)

where, using the convention \(\begin{pmatrix} r \\ -|s| \end{pmatrix} = 0\) for a binomial coefficient with negative down entry,

\[
A = \frac{|S_{h_f}|^2}{N} \sum_{k=0}^{N-2} f_k^2 \left( \begin{array}{c} N-1 \\ k \end{array} \right) \left( \begin{array}{c} N-3 \\ k-1 \end{array} \right) 
\]

(A9)

\[
B = \frac{1}{N} \sum_{k=0}^{N-2} f_k^2 \left( \begin{array}{c} N-1 \\ k \end{array} \right) \left( \begin{array}{c} N-2 \\ k \end{array} \right) - \left( \begin{array}{c} N-3 \\ k-1 \end{array} \right) \right) 
\]

(A10)

and \(C_{1,1}(r)\) is the \((1,1)\) algebraic complement of the matrix \(T(\mathbf{r})\) whose determinant is equal to one for even \(x + y\). The \((1,1)\) algebraic complement can be expressed in terms of the \((1,1)\) element of the matrix \(T(\mathbf{r})\):

\[
C_{1,1}(r) = T^T(\mathbf{r})_{1,1} \text{Det}[T(\mathbf{r})] = T(\mathbf{r})_{1,1} \text{ (since } T(\mathbf{r})_{i,j} \in \mathbb{R}) \text{). Next one has to recognize that } T(\mathbf{r})_{1,1} \text{ is, by
definition, equal to \( t_1(r) \) (see Eq.\( (46) \)) whose analytic expression is given in Eq.\( (53) \). Therefore, any time \( x+y \) is even we have

\[
X(r) = \frac{1}{|\delta_{ij}|^2} [A + B \times T_0(r)]^2
\]  

(A11)

On the other hand, for odd \( x+y \) the translation matrix in the local basis is antiblock diagonal, that is

\[
\tilde{T}(r) c_i^0 |0\rangle = \sum_{\gamma=1}^{2N^2-2} T(r)_{i,\gamma} c_i^0 |0\rangle = \begin{cases} \sum_{\alpha=N}^{2N^2-2} T(r)_{i,\alpha} c_i^0 |0\rangle, & i = 1, \ldots, N - 1 \\ \sum_{\beta=1}^{N} T(r)_{i,\beta} c_i^0 |0\rangle, & i = N, \ldots, 2N - 2 \end{cases}
\]  

(A12)

and hence

\[
\tilde{T}(r) c_i^0 |\Phi^0_\downarrow\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha_1=1}^{N-1} \sum_{\alpha_{N-1}=1}^{\alpha_1} \prod_{a=1}^{N-1} T(r)_{\alpha,a} \prod_{b=N}^{2N-2} T(r)_{b,b} \times
\]

\[
\sum_{k=0}^{N-2} (-1)^k f_k \sum_{i_k > \ldots > i_2 = 2 \ldots > i_1 = 1} \langle 0|c_{N-1,1} c_{i_1,\ldots,1} S_{m_{N-2},k} \ldots S_{m_1,1} S_{j_{N-1,1}}^\dagger c_{i_1,\ldots,1}^\dagger |0\rangle \times
\]

\[
\times \{ \sum_{m_{N-2} > \ldots > m_2 = 2 \ldots > j_1 = 1} \langle 0|c_{N-2,2,\ldots,1} S_{m_{N-2},k} \ldots S_{m_1,1} S_{j_{N-1,1}}^\dagger c_{i_1,\ldots,1}^\dagger c_{N-1,1}^\dagger |0\rangle \}
\]  

(A13)

Let us consider the \( k \)-th term of this state. One can check by direct inspection that the only non-vanishing contribution in the scalar product with the state \( c_{i_1,\ldots,1}^\dagger |\Phi^0_\downarrow\rangle \) comes from the \( (N-k-2) \)-th term of the corresponding expansion, see Eq.\((50)\). Hence

\[
X(r) = -\frac{1}{N} \sum_{\alpha_1=1}^{N-1} \sum_{\alpha_{N-1}=1}^{\alpha_1} \prod_{a=1}^{N-1} T(r)_{\alpha,a} \prod_{b=N}^{2N-2} T(r)_{b,b} \times
\]

\[
\sum_{k=0}^{N-2} (-1)^k f_k \sum_{i_k > \ldots > i_2 = 2 \ldots > i_1 = 1} \langle 0|c_{N-1,1} c_{i_1,\ldots,1} S_{m_{N-2},k} \ldots S_{m_1,1} S_{j_{N-1,1}}^\dagger c_{i_1,\ldots,1}^\dagger |0\rangle \times
\]

\[
\times \{ \sum_{m_{N-2} > \ldots > m_2 = 2 \ldots > j_1 = 1} \langle 0|c_{N-2,2,\ldots,1} S_{m_{N-2},k} \ldots S_{m_1,1} S_{j_{N-1,1}}^\dagger c_{i_1,\ldots,1}^\dagger c_{N-1,1}^\dagger |0\rangle \}
\]  

(A14)

Analogously to the case \( x+y \) even, the particular structure of \( |\Phi^0_\uparrow\rangle \) allows the following simplification

\[
\sum_{j_{N-1} > \ldots > j_1 = 1} \langle 0|c_{N-1,1} c_{i_1,\ldots,1} S_{m_{N-2},k} \ldots S_{m_1,1} S_{j_{N-1,1}}^\dagger c_{i_1,\ldots,1}^\dagger |0\rangle = \varepsilon_{j_1,\ldots,j_{N-1}} \sum_{j_{N-1} > \ldots > j_1 = 1} \langle 0|c_{N-1,1} c_{i_1,\ldots,1} S_{m_{N-2},k} \ldots S_{m_1,1} S_{j_{N-1,1}}^\dagger c_{i_1,\ldots,1}^\dagger |0\rangle + \ldots
\]  

(A15)

where \( \varepsilon_{\alpha_1,\ldots,\alpha_{N-1}} = \varepsilon_{\alpha_1-1,\ldots,\alpha_{N-1}-1,\alpha_{N+1}} \) and the sum on the right hand side of Eq.\((16)\) means that the indices \( i_k > \ldots > i_1 \) run in the interval \( \{N, \ldots, 2N-2\} \) in such a way that no of them is equal to \( \alpha_1 \). All the neglected terms contribute nothing to the scalar product.

Using Eq.\((15)\) the second row of Eq.\((14)\) yields

\[
\varepsilon_{j_1,\ldots,j_{N-1}} \sum_{m_{N-2} > \ldots > m_2 = 2 \ldots > j_1 = 1} \langle 0|c_{N-1,1} c_{i_1,\ldots,1} S_{m_{N-2},k} \ldots S_{m_1,1} S_{j_{N-1,1}}^\dagger c_{i_1,\ldots,1}^\dagger |0\rangle = \varepsilon_{j_1,\ldots,j_{N-1}} \left( \frac{N-2}{k} \right)
\]  

(A17)

while using Eq.\((16)\) the third row of Eq.\((14)\) yields

\[
\varepsilon_{\alpha_1,\ldots,\alpha_{N-1}} \sum_{n_{N-2} > \ldots > n_1 = N \ldots > i_1 = N} \langle 0|c_{N-2,2,\ldots,1} S_{n_{N-2},k} \ldots S_{n_1,1} S_{i_1,\ldots,1} S_{n_{N-1,1}}^\dagger c_{n_{N-1,1},\ldots,1}^\dagger c_{N-2,1}^\dagger |0\rangle = \varepsilon_{\alpha_1,\ldots,\alpha_{N-1}} \left( \frac{N-2}{k} \right)
\]  

(A18)
Substituting these results in the expression for \( X(r) \) we get

\[
X(r) = -\frac{C}{|S_h|^2} = -\frac{1}{|S_h|^2} [A + B \times (4N - 4)]
\]

(A19)

where we have taken into account that \( \text{Det}[T(r)] = -1 \) for odd \( x + y \) and the constant \( C \) is given by

\[
C = \frac{|S_h|^2}{N} \sum_{k=0}^{N-2} f_k f_{N-k-2} \left( \frac{N-2}{k} \right)^2.
\]

(A20)

In the last equality of Eq.(A19) we have used \( C = A + B \times (4N - 4) \) which is a direct consequence of the sum rule for the spin correlation function, see Eq.(58).

**APPENDIX B: EVALUATION OF Y**

Here we show that \( Y(r) \equiv \langle \Phi^{[0]}_\uparrow | \hat{T}(r) | \Phi^{[0]}_\downarrow \rangle \) has the form shown in Eq.(80) and we derive the explicit values for the two constants \( D \) and \( E \). As for \( X(r) \) we will first consider the case \( x + y \) even and thereafter the case \( x + y \) odd. Making use of Eq.(A1), we get

\[
\hat{T}(r)|\Phi^{[0]}_\uparrow \rangle = \frac{1}{\sqrt{N}} \sum_{\alpha_1..\alpha_{N-1}=1}^{N-1} \sum_{\beta_1..\beta_{N-1}=N}^{N} \prod_{a=1}^{2N-2} T(r)_{a,a} \prod_{b=N}^{2N-2} T(r)_{b,b} \times
\]

\[
\times \sum_{k=0}^{N-2} (-1)^k f_k \sum_{i_k > .. > i_2 > j_k > .. > j_1 = 1} \tilde{S}_{\alpha_{i_k}}^{\uparrow} \cdots \tilde{S}_{\alpha_{i_2}}^{\uparrow} \tilde{S}_{\beta_{j_k}}^{\downarrow} \cdots \tilde{S}_{\beta_{j_1}}^{\downarrow} \tilde{c}^\dagger_{\alpha_{N-1}} \cdots \tilde{c}^\dagger_{\alpha_{1}} |0\rangle
\]

(B1)

The \( k \)-th term in the sum of Eq.(B1) gives non-vanishing scalar product only with the \( k \)-th term in Eq.(49) and hence

\[
Y(r) = \frac{1}{N} \sum_{\alpha_1..\alpha_{N-1}=1}^{N-1} \sum_{\beta_1..\beta_{N-1}=N}^{N} \prod_{a=1}^{2N-2} T(r)_{a,a} \prod_{b=N}^{2N-2} T(r)_{b,b} \sum_{k=0}^{N-2} f_k ^2 \times
\]

\[
\times \{ \sum_{m_k > .. > m_2 = 2} \sum_{i_k > .. > i_1 = 2} |0\rangle c_{N-1,\uparrow} c_{N-1,\downarrow} \tilde{S}_{m_k}^{\uparrow} \cdots \tilde{S}_{m_2}^{\uparrow} \tilde{S}_{\alpha_{i_k}}^{\uparrow} \cdots \tilde{S}_{\alpha_{i_2}}^{\uparrow} \tilde{c}^\dagger_{\alpha_{N-1}} \cdots \tilde{c}^\dagger_{\alpha_{1}} |0\rangle \} \times
\]

\[
\times \{ \sum_{n_k > .. > n_2 = 2} \sum_{j_k > .. > j_1 = 2} |0\rangle c_{2N-2,\uparrow} c_{2N-2,\downarrow} \tilde{S}_{n_k}^{\uparrow} \cdots \tilde{S}_{n_2}^{\uparrow} \tilde{S}_{\beta_{j_k}}^{\downarrow} \cdots \tilde{S}_{\beta_{j_1}}^{\downarrow} \tilde{c}^\dagger_{\beta_{N-1}} \cdots \tilde{c}^\dagger_{\beta_{1}} \downarrow |0\rangle \}.
\]

(B2)

Now we use the fact that the indices \( \alpha_1, \ldots, \alpha_{N-1} \) must be all different and within the range \( \{1, \ldots, N-1\} \) otherwise the scalar product vanishes. This means that

\[
\sum_{i_k > .. > i_1 = 2} \tilde{S}_{\alpha_{i_k}}^{\uparrow} \cdots \tilde{S}_{\alpha_{i_2}}^{\uparrow} \tilde{c}^\dagger_{\alpha_{N-1}} \cdots \tilde{c}^\dagger_{\alpha_{1}} |0\rangle = \varepsilon_{\alpha_1..\alpha_{N-1}} \sum_{i_k > .. > i_1 = 1} \tilde{S}_{i_1}^{-\uparrow} \cdots \tilde{S}_{i_k}^{-\uparrow} \cdots \tilde{c}^\dagger_{\alpha_{N-1}} \cdots \tilde{c}^\dagger_{\alpha_{1}} |0\rangle + \ldots
\]

(B3)

where the neglected terms do not contribute to the scalar product. In the second row of Eq.(B2), \( c_{i,\uparrow} \) commutes with all the raising spin operators whatever are the values of the \( k \) indices \( m_k > .. > m_1 \) in the range specified by the sum. This implies that \( i_1 \) cannot be 1. On the other hand \( c_{i,\downarrow} \) commutes with all the lowering spin operators and hence no one of the indices \( m_k > .. > m_1 \) can be \( \alpha_1 \) otherwise the corresponding term vanishes. Hence the term in the second row gives

\[
\sum_{m_k > .. > m_1 = 2} \sum_{i_k > .. > i_1 = 2} \varepsilon_{\alpha_1..\alpha_{N-1}} |0\rangle c_{N-1,\uparrow} c_{N-1,\downarrow} \tilde{S}_{m_k}^{\uparrow} \cdots \tilde{S}_{m_2}^{\uparrow} \tilde{S}_{\alpha_{i_k}}^{\uparrow} \cdots \tilde{S}_{\alpha_{i_2}}^{\uparrow} \tilde{c}^\dagger_{\alpha_{N-1}} \cdots \tilde{c}^\dagger_{\alpha_{1}} |0\rangle =
\]

\[
= \sum_{i_k > .. > i_1 = 2} |0\rangle \varepsilon_{\alpha_1..\alpha_{N-1}}.
\]

(B4)

If \( k = N - 2 \) the sum is zero except for \( \alpha_1 = 1 \) since the indices \( i_k > .. > i_1 \) don't have space to run. Hence
while the third row of Eq.(B2) yields
\[
\hat{\varepsilon}_{\beta_1 \ldots \beta_{N-1}} \sum_{n_k \geq \ldots \geq n_1 = N \ j_k \geq \ldots \geq j_1 = N} (0|c_{2N-2,k} \ldots c_{N,k}|\hat{S}_{n_k}^- \ldots \hat{S}_{n_1}^- \hat{S}_{j_k}^+ \ldots \hat{S}_{j_1}^+ c_{N,k}^\dagger \ldots c_{2N-2,k}^\dagger |0) = \\
\hat{\varepsilon}_{\beta_1 \ldots \beta_{N-1}} \left( \begin{array}{c} N - 1 \\ k \end{array} \right)
\]  
(B6)
as can be verified by using the total antisymmetry of each homogeneous polynomial in the raising spin operators.

Therefore for even \(x + y\) one can write
\[
Y(r) = \frac{1}{4} + \frac{D}{|S_{k,r}|^2} + EC_{1,1}(r)T(r)_{1,1} = \frac{1}{4} + \frac{1}{|S_{k,r}|^2} [D + E \times T_{h1}(r)^2],
\]  
(B7)
where \(D\) and \(E\) are two \(N\)-dependent constants given by:
\[
D = \frac{|S_{k,r}|^2}{N} \left[ \sum_{k=0}^{N-3} f_k^2 \left( \begin{array}{c} N - 1 \\ k \end{array} \right) \left( \begin{array}{c} N - 3 \\ k \end{array} \right) - \frac{N}{4} \right]
\]  
(B8)
\[
E = \frac{1}{N} \left\{ (N - 1)f_{k-2}^{N-2} + \sum_{k=1}^{N-3} f_k^2 \left( \begin{array}{c} N - 1 \\ k \end{array} \right) \left[ \left( \begin{array}{c} N - 2 \\ k \end{array} \right) - \left( \begin{array}{c} N - 3 \\ k \end{array} \right) \right] \right\}
\]  
(B9)

For odd \(x + y\) we make use of Eq.(A12). Then, the action of \(\hat{T}(r)\) over \(|\Phi_1^{(0)}\rangle\) gives
\[
\hat{T}(r)|\Phi_1^{(0)}\rangle = \frac{1}{\sqrt{N}} \sum_{\alpha_1 \ldots \alpha_{N-1} = N} \sum_{\beta_1 \ldots \beta_{N-1} = 1} T(r)_{a,a} \prod_{b=N}^{2N-2} T(r)_{b,b} \times \\
\sum_{k=0}^{N-2} (-)^k f_k \sum_{i_k \geq \ldots \geq i_1 = 2} \sum_{j_k \geq \ldots \geq j_1 = 1} \hat{S}_{i_k}^- \ldots \hat{S}_{i_1}^- \hat{S}_{j_k}^+ \ldots \hat{S}_{j_1}^+ c_{\alpha_1}^\dagger \ldots c_{\alpha_{N-1}}^\dagger c_{\beta_1}^\dagger \ldots c_{\beta_{N-1}}^\dagger |0\rangle.
\]  
(B10)

In the scalar product with the \(|\Phi_2^{(0)}\rangle\) state, only the terms with the same number of up (or down) spins in the first \(N - 1\) (and hence in the last \(N - 1\)) local states will survive. Let us consider for example the \(k\)-th term of the sum in the second row of Eq.(B10); it contains states where \(k\) of the last \(N - 1\) local states have spin down and \(k\) of the first \(N - 1\) local states have spin up. This term has non-vanishing scalar product only with the \((N - k - 1)\)-th term of the sum in the definition of \(|\Phi_2^{(0)}\rangle\), Eq.(49). In particular this implies that the terms where the first and the last \(N - 1\) local states have all the spins aligned do not contribute to the scalar product. Hence
\[
Y(r) = \frac{1}{N} \sum_{\alpha_1 \ldots \alpha_{N-1} = N} \sum_{\beta_1 \ldots \beta_{N-1} = 1} T(r)_{a,a} \prod_{b=N}^{2N-2} T(r)_{b,b} \sum_{k=1}^{N-2} f_k f_{N-k-1} \times \\
\times \{ \sum_{m_{N-k-1} > \ldots > m_1 = 2} T^{(0)}_{m_{N-k-1},\ldots,m_1} \hat{S}_{m_{N-k-1}}^+ \ldots \hat{S}_{m_1}^+ \hat{S}_{N-k-1}^- \ldots \hat{S}_{N-k}^- |0\rangle \} \times \\
\times \{ \sum_{n_{N-k-1} > \ldots > n_1 = 1} |0\rangle c_{2N-2,k} \ldots c_{N,k} |\hat{S}_{n_{N-k-1}}^- \ldots \hat{S}_{n_1}^- \hat{S}_{N,k}^+ \ldots \hat{S}_{N-k}^+ c_{N,k}^\dagger \ldots c_{2N-2,k}^\dagger |0\rangle \}.
\]  
(B11)

Let us consider the term in the second row. For a given choice of \(\beta_1 \ldots \beta_{N-1}\) one finds
\[
\sum_{j_k \geq \ldots \geq j_1 = 1} \hat{S}_{j_k}^+ \ldots \hat{S}_{j_1}^+ c_{\beta_1}^\dagger \ldots c_{\beta_{N-1}}^\dagger |0\rangle = \hat{\varepsilon}_{\beta_1 \ldots \beta_{N-1}} \sum_{j_k \geq \ldots \geq j_1 = 1} \hat{S}_{j_k}^+ \ldots \hat{S}_{j_1}^+ c_{\alpha_1}^\dagger \ldots c_{\alpha_{N-1}}^\dagger |0\rangle + \ldots,
\]  
(B12)
where the missed terms do not contribute to the scalar product. Since the $c_{1\uparrow}$ annihilation operator commutes with all the raising spin operators coming from the sum over $m_{N-k-1} \ldots > m_1$, $j_1$ is constrained to be 1 for all non-vanishing contributions. Still for $j_k \ldots > j_2$ fixed there is only one choice for $m_{N-k-1} \ldots > m_1$ to have non-vanishing result. In particular, the possible results for a given choice of $j_k \ldots > j_2$ and $m_{N-k-1} \ldots > m_1$ are 0 or 1. Hence the term in the first square bracket yields

$$
\varepsilon_{\beta_1 \ldots \beta_{N-1}} \sum_{m_{N-k-1} \ldots > m_1=2}^{N-1} \sum_{j_k \ldots > j_2=2}^{N-1} \langle 0 | c_{N-1,\uparrow} \ldots c_{1,\uparrow} S_{m_{N-k-1},\downarrow} \ldots S_{m_1,\downarrow} j_k \ldots S_{j_1,\downarrow} \ldots c_{N-1,\downarrow} | 0 \rangle =
\varepsilon_{\beta_1 \ldots \beta_{N-1}} \binom{N-2}{k-1}.
$$

(B13)

A similar trick can be used for the term in the third row of Eq.(B11). We get

$$
\sum_{i_k \ldots > i_1=2}^{N-1} \sum_{i_k \ldots > i_1=N, \neq \alpha_1}^{2N-2} \langle 0 | c_{2N-2,\downarrow} \ldots c_{N,\downarrow} S_{N-k-1,\downarrow} \ldots S_{\alpha_1,\downarrow} i_k \ldots S_{i_1,\downarrow} \ldots c_{2N-2,\downarrow} | 0 \rangle =
\binom{N-2}{k} \varepsilon_{\alpha_1 \ldots \alpha_{N-1}}.
$$

(B14)

Since the $c_{i_1,\downarrow}$ creation operator commutes with all the lowering spin operators coming from the sum over $i_k \ldots > i_1$, one of the indices $n_{N-k-1} \ldots > n_1$ is constrained to be $\alpha_1$ and the third row of Eq.(B11) can be rewritten as

$$
\varepsilon_{\alpha_1 \ldots \alpha_{N-1}} \sum_{m_{N-k-1} \ldots > m_1=2}^{2N-2} \sum_{n_{N-k-1} \ldots > n_1=2}^{2N-2} \langle 0 | c_{2N-2,\downarrow} \ldots c_{N,\downarrow} S_{N-k-1,\downarrow} \ldots S_{\alpha_1,\downarrow} i_k \ldots S_{i_1,\downarrow} \ldots c_{2N-2,\downarrow} | 0 \rangle =
\binom{N-2}{k} \varepsilon_{\alpha_1 \ldots \alpha_{N-1}}.
$$

(B15)

Substituting these results in Eq.(B11) one obtains

$$
Y(r) = \frac{F_N}{|S_{\alpha,\uparrow}|^2} \equiv \frac{1}{N^2} \binom{D + E \times (4N - 4)}{D + E \times (4N - 4)}
$$

(B16)

where we have taken into account that $\text{Det}[T(r)] = -1$ for odd $x + y$ and the constant $F_N$ is given by

$$
F_N = \frac{|S_{\alpha,\uparrow}|^2}{N} \sum_{k=1}^{N-2} \frac{\binom{N-2}{k} \binom{N-2}{k-1}}{k!}.
$$

(B17)

In the last equality of Eq.(B16) we have used $F_N = |S_{\alpha,\uparrow}|^2/4 - D - E \times (4N - 4)$ which is a direct consequence of the sum rule for the charge correlation function, see Eq.(81).

REFERENCES

[1] Elliot Lieb, Phys. Rev. Lett. 62, 1201 (1989).
[2] Cheng Ning Yang, Phys. Rev. Lett. 63, 2144 (1989).
[3] Cheng Ning Yang and S. C. Zhang, Mod. Phys. Lett. B 4, 759 (1990).
[4] B. Friedman, Europhys. Lett. 14 (5), 495 (1991).
[5] J. Galan and J. A. Verges, Phys. Rev. B 44, 10093 (1991).
[6] Michele Cini and Gianluca Stefanucci, J. Phys.: Condens. Matter 13, 1279 (2001).
[7] Michele Cini and Gianluca Stefanucci, Solid State Communications 117, 451 (2001).
[8] A. Moreo and E. Dagotto, Phys. Rev. B 41, 9488 (1990).
[9] K. Kobayashi and K. Iguchi, Phys. Rev. B 40, 7073 (1989).
[10] J. G. Bednorz and K. A. M"uller, Z. Phys. B 64, 189 (1986).
[11] Efthimios Kaxiras and Efstratios Manousakis, Phys. Rev. B 37, 656 (1988).
[12] Florian Gebhard and Dieter Vollhardt, Phys. Rev. B 38, 6911 (1988).
[13] S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh Jr., J. E. Gubernatis and R. T. Scalettar, Phys. Rev. B 40, 506 (1989).
[14] Z. B. Huang, H. Q. Lin and J. E. Gubernatis, Phys. Rev. B 63, 115112-1 (2001).
[15] Y. M. Vilk, Liang Chen and A. M. S. Tremblay, Phys. Rev. B 49, 13267 (1994).
[16] G. Fano, F. Ortolani and A. Parola, Phys. Rev. B 46, 1048 (1992).
[17] G. Fano, F. Ortolani and A. Parola, Phys. Rev. B 43, 6877 (1990).
[18] Guang Shan Tian, Phys. Rev. B 63, 224413 (2001).
[19] M. Cini, E. Perfetto and G. Stefanucci, Eur. Phys. J. B 20, 91 (2001).
[20] W. Metzner and D. Vollhardt, Phys. Rev. B 39, 4462 (1989).