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# Analytic correlation functions of the two-dimensional half-filled Hubbard model at weak coupling

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**Abstract**

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

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

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 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 $\boldsymbol{r}$, $\boldsymbol{r}'$ the spatial degrees of freedom of the creation and annihilation operators $c^{\dagger}$ and $c$ respectively. The sum on $\langle \boldsymbol{r}, \boldsymbol{r}' \rangle$ is over the pairs of nearest-neighbour sites and $\hat{n}_{r\sigma}$ is the number operator on site $\boldsymbol{r}$ 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

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

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

$\boldsymbol{T}$ and hence under the space group $\boldsymbol{G} = \boldsymbol{T} \otimes C_{4v}$; $\otimes$ means the semidirect product. The presence of spin and pseudospin symmetries [1] leads to SO(4) group [2, 3]; below, we shall work in the subspace of vanishing spin and pseudospin. We represent sites by $\boldsymbol{r} = (x, y)$ and wavevectors by $\boldsymbol{k} = (k_x, k_y) = (2\pi/N)(x, y)$, with $x, y = 0, \ldots, N-1$. In terms of the Fourier expanded fermion operators $c_{\boldsymbol{k}\sigma} = (1/N)\sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{r}\sigma}$, we have $H_0 = \sum_{\boldsymbol{k}} \epsilon(\boldsymbol{k}) c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$ with $\epsilon(\boldsymbol{k}) = 2t[\cos k_x + \cos k_y]$. Then the one-body plane wave state $c^{\dagger}_{\boldsymbol{k}\sigma}|0\rangle \equiv |\boldsymbol{k}\sigma\rangle$ 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 $\binom{2N-2}{N-1}^2$ 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 wavefunction $|\Psi^{[0]}_{AF}\rangle$ 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 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 $|\Psi^{[0]}_{AF}\rangle$ clearly deserves further study: although it is an eigenstate only at the first order in $U$, it must represent a good many of the properties of the full ground state. Here we wish to show that the same *local* formalism that allows one to build $|\Psi^{[0]}_{AF}\rangle$ 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

$$G_{\mathrm{charge}}(\boldsymbol{r}) \equiv \langle\Psi^{[0]}_{AF}|\hat{n}_{\boldsymbol{r}}\hat{n}_0|\Psi^{[0]}_{AF}\rangle \tag{2}$$

for the charge correlation function and

$$G_{\mathrm{spin}}(\boldsymbol{r}) \equiv \langle\Psi^{[0]}_{AF}|\hat{\boldsymbol{S}}_{\boldsymbol{r}} \cdot \hat{\boldsymbol{S}}_0|\Psi^{[0]}_{AF}\rangle \tag{3}$$

for the spin one. Here $\hat{n}_{\boldsymbol{r}}$ is the number operator and $\hat{\boldsymbol{S}}_{\boldsymbol{r}}$ is the spin vector operator at site $\boldsymbol{r}$; the subscripts 0 denote the site at the origin.

Studies [9] of correlation functions in the three-band Hubbard model were aimed at the characterization of possible pairing mechanisms shortly 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 one-dimensional 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 2, we go over in section 3 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 4 and the charge one in section 5. The results are discussed and compared with available data in section 6.

## 2. 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 $\boldsymbol{k}$ wavevectors such that $\epsilon(\boldsymbol{k}) = 0$. At half filling ($N^2$ particles) for $U = 0$ the $\mathcal{S}_{hf}$ shell is half occupied, while all $|\boldsymbol{k}\rangle$ orbitals such that $\epsilon(\boldsymbol{k}) < 0$ are filled. The $\boldsymbol{k}$ 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,

$$\hat{S}^z = \tfrac{1}{2}\sum_{\boldsymbol{r}}(\hat{n}_{\boldsymbol{r}\uparrow} - \hat{n}_{\boldsymbol{r}\downarrow}), \qquad \hat{S}^+ = \sum_{\boldsymbol{r}} c^\dagger_{\boldsymbol{r}\uparrow} c_{\boldsymbol{r}\downarrow}, \qquad \hat{S}^- = (\hat{S}^+)^\dagger, \tag{4}$$

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

It can be shown [6] that the structure of the first-order wavefunctions 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 $\boldsymbol{G}$ symmetry. Any plane-wave state $\boldsymbol{k}$ belongs to a one-dimensional irrep of $\boldsymbol{T}$; moreover, it also belongs to a *star* of $\boldsymbol{k}$ vectors connected by operations of $\mathrm{C_{4v}}$, and one member of the star has $k_x \geqslant k_y \geqslant 0$. We recall that any $\boldsymbol{k} \in \mathcal{S}_{hf}$ lies on a square with vertices on the axes at the Brillouin zone boundaries. Choosing an arbitrary $\boldsymbol{k} \in \mathcal{S}_{hf}$ with $k_x \geqslant k_y \geqslant 0$, hence $k_x + k_y = \pi$, the set of vectors $R_i\boldsymbol{k} \in \mathcal{S}_{hf}$, where $R_i \in \mathrm{C_{4v}}$, is a basis for an irrep of $\boldsymbol{G}$. The high-symmetry vectors $\boldsymbol{k}_A = (\pi, 0)$ and $\boldsymbol{k}_B = (0, \pi)$ are the basis of the only two-dimensional irrep of $\boldsymbol{G}$, which exists for any $N$. If $N/2$ is even, one also finds the high-symmetry wavevectors $\boldsymbol{k} = (\pm\pi/2, \pm\pi/2)$ which mix among themselves under $\mathrm{C_{4v}}$ operations and yield a four-dimensional irrep. In general, when $\boldsymbol{k}$ is not in a special symmetry direction, the vectors $R_i\boldsymbol{k}$ are all different, so all the other irreps of $\boldsymbol{G}$ have dimension eight, the number of operations of the point group $\mathrm{C_{4v}}$.

Below, we shall need the number of these irreps. Since eight times the number of eight-dimensional irreps plus four times that of four-dimensional ones plus two 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 eight if $N/2$ is even and $N_o = \frac{1}{2}(N/2 - 1)$ irreps of dimension eight if $N/2$ is odd.

In this way, $\mathcal{S}_{hf}$ is seen to be the union of disjoint bases of irreps of the space group. This break-up of $\mathcal{S}_{hf}$ enables us to define a *real* symmetry-adapted one-body *local* basis which allows us to carry on the analysis for any $N$.

The one-body *local* basis is obtained by projecting onto the irreps of $\mathrm{C_{4v}}$ the $|\boldsymbol{k}\rangle$ states of $\mathcal{S}_{hf}$ that belong to a given irrep of $\boldsymbol{G}$. As already noted, $\boldsymbol{k}_A = (\pi, 0)$ and $\boldsymbol{k}_B = (0, \pi)$ belong to $\mathcal{S}_{hf}$ and are the basis of a two-dimensional irrep of $\boldsymbol{G}$. Let

$$|\psi''_{A_1}\rangle = \frac{1}{\sqrt{2}}(|\boldsymbol{k}_A\rangle + |\boldsymbol{k}_B\rangle), \qquad |\psi''_{B_1}\rangle = \frac{1}{\sqrt{2}}(|\boldsymbol{k}_A\rangle - |\boldsymbol{k}_B\rangle) \tag{5}$$

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

For even $N/2$, $\mathcal{S}_{hf}$ also comprises the basis wavevectors $\boldsymbol{k}_1 = (\pi/2, \pi/2)$, $\boldsymbol{k}_2 = (-\pi/2, \pi/2)$, $\boldsymbol{k}_3 = (\pi/2, -\pi/2)$, $\boldsymbol{k}_4 = (-\pi/2, -\pi/2)$ of the four-dimensional irrep of $\boldsymbol{G}$.

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

$$|\psi'_I\rangle = \sum_{i=1}^{4} O'_{Ii}|\boldsymbol{k}_i\rangle, \tag{6}$$

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

$$O' = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ \mathrm{i} & -\mathrm{i} & \mathrm{i} & -\mathrm{i} \\ \mathrm{i} & \mathrm{i} & -\mathrm{i} & -\mathrm{i} \end{bmatrix}. \tag{7}$$

For $N > 4$, $\mathcal{S}_{hf}$ also contains $\boldsymbol{k}$ vectors that are away from special symmetry directions. These form eight-dimensional irreps of $\boldsymbol{G}$ since $R_i\boldsymbol{k}$ are all different for all $R_i \in C_{4v}$. In other terms, any eight-dimensional irrep of $\boldsymbol{G}$ 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 $\boldsymbol{k}^{[m]} = (k_x^{[m]}, k_y^{[m]})$ with $k_x^{[m]} \geqslant k_y^{[m]} \geqslant 0$ be a wavevector of the $m$th eight-dimensional irrep of $\boldsymbol{G}$ and let $R_i$, $i = 1, \ldots, 8$ denote respectively the identity $\mathbf{1}$, the anticlockwise and clockwise $90^\circ$ rotation $C_4^{(+)}$, $C_4^{(-)}$, the $180^\circ$ 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

$$|\psi_I^{[m]}\rangle = \sum_{i=1}^{8} O_{Ii}|R_i\boldsymbol{k}^{[m]}\rangle, \tag{8}$$

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

$$O = \frac{1}{\sqrt{8}}\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 \\ \mathrm{i} & \mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} \\ \mathrm{i} & -\mathrm{i} & \mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} & -\mathrm{i} & \mathrm{i} \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 \\ \mathrm{i} & -\mathrm{i} & \mathrm{i} & -\mathrm{i} & \mathrm{i} & -\mathrm{i} & \mathrm{i} & -\mathrm{i} \\ \mathrm{i} & \mathrm{i} & -\mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} & \mathrm{i} & -\mathrm{i} \end{bmatrix}. \tag{9}$$

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:

$$|\Phi_{AF}\rangle_\sigma \equiv \left|\left(\prod_{m=1}^{N_e} \psi_{A_1}^{[m]}\psi_{B_2}^{[m]}\psi_{E_x}^{[m]}\psi_{E_y}^{[m]}\right)\psi'_{A_1}\psi'_{B_2}\psi''_{A_1}\right\rangle_\sigma \otimes\left|\left(\prod_{m=1}^{N_e} \psi_{A_2}^{[m]}\psi_{B_1}^{[m]}\psi_{E'_x}^{[m]}\psi_{E'_y}^{[m]}\right)\psi'_{E_x}\psi'_{E_y}\psi''_{B_1}\right\rangle_{-\sigma} \tag{10}$$

for even $N/2$ and

$$|\Phi_{AF}\rangle_\sigma \equiv \left|\left(\prod_{m=1}^{N_o} \psi_{A_1}^{[m]}\psi_{B_2}^{[m]}\psi_{E_x}^{[m]}\psi_{E_y}^{[m]}\right)\psi''_{A_1}\right\rangle_\sigma \otimes \left|\left(\prod_{m=1}^{N_o} \psi_{A_2}^{[m]}\psi_{B_1}^{[m]}\psi_{E'_x}^{[m]}\psi_{E'_y}^{[m]}\right)\psi''_{B_1}\right\rangle_{-\sigma} \tag{11}$$

for odd $N/2$, with $\sigma = \uparrow, \downarrow$. In [6, 7] we have shown the following.

- $|\Phi_{AF}\rangle_\sigma$ is an eigenstate of $\hat{W}$ with vanishing eigenvalue ($W = 0$ *state*).
- Under a lattice step translation $|\Phi_{AF}\rangle_\sigma \to -|\Phi_{AF}\rangle_{-\sigma}$. Therefore, it manifestly shows an antiferromagnetic order (*antiferromagnetic property*).
- Introducing the projection operator $P_S$ on the spin $S$ subspace, one finds that $P_S|\Phi_{AF}\rangle_\sigma \equiv |\Phi_{AF}^{[S]}\rangle \neq 0,\ \forall S = 0, \ldots, N-1$. Then, $\langle\Phi_{AF}|\hat{W}|\Phi_{AF}\rangle = \sum_{S=0}^{N-1} \langle\Phi_{AF}^{[S]}|\hat{W}|\Phi_{AF}^{[S]}\rangle = 0$, 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 and 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
$$E_U \equiv \frac{\langle\Phi_{AF}^{[0]}|\hat{W}|\Phi_{AF}^{[0]}\rangle}{N^2} = \frac{U}{4} - U\frac{(N-1)^2}{N^4}. \tag{12}$$
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 $N^2$ particles 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 this. 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].

## 3. 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

$$\begin{aligned} c_{r\downarrow} &= d_{r\downarrow} \\ c_{r\uparrow} &= (-)^{x+y} d_{r\uparrow}^\dagger, \end{aligned} \qquad r = (x, y). \tag{13}$$

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

$$H = t\sum_\sigma \sum_{\langle r,r'\rangle} d_{r\sigma}^\dagger d_{r'\sigma} - \sum_r U\hat{n}_{r\uparrow}^{(d)}\hat{n}_{r\downarrow}^{(d)} + U\hat{N}_\downarrow^{(d)}, \qquad U > 0, \tag{14}$$

with $\hat{n}_{r\sigma}^{(d)} = d_{r\sigma}^\dagger d_{r\sigma}$ and $\hat{N}_\sigma^{(d)} = \sum_r \hat{n}_{r\sigma}^{(d)}$. 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 $d_r^\dagger$ with real coefficients acting on the vacuum), we recall that the ground state at half filling

$$|\Psi^{[0]}\rangle = \sum_{\Gamma_1\Gamma_2} L_{\Gamma_1\Gamma_2}|\Psi_{\Gamma_1\uparrow}\rangle \otimes |\Psi_{\Gamma_2\downarrow}\rangle \tag{15}$$

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

In this section we shall perform the unitary particle–hole transformation in equation (13) on the ground state of equations (10) and (11). We shall 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 $|\Phi_{AF}\rangle_\sigma$ (equations (10) and (11)). We write $|\Phi_{AF}\rangle_\sigma$ as

$$|\Phi_{AF}\rangle_\sigma = c_{1,\sigma}^\dagger \ldots c_{N-1,\sigma}^\dagger c_{N,-\sigma}^\dagger \ldots c_{2N-2,-\sigma}^\dagger |0\rangle. \tag{16}$$

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

$$\begin{aligned}|\Phi_{AF}^{[0]}\rangle &= P_{S=0}|\Phi_{AF}\rangle_\uparrow \\ &= \frac{1}{\sqrt{\mathcal{N}}}\left\{\sum_{k=N/2}^{1}(-)^k g_k \sum_{i_{\frac{N}{2}-k}>\cdots>i_1=1}^{N-1}\hat{S}_{i_1}^-\ldots\hat{S}_{i_{\frac{N}{2}-k}}^- \sum_{j_{\frac{N}{2}-k}>\cdots>j_1=N}^{2N-2}\hat{S}_{j_1}^+\ldots\hat{S}_{j_{\frac{N}{2}-k}}^+\right\} \\ &\quad\times c_{1,\uparrow}^\dagger\ldots c_{N-1,\uparrow}^\dagger c_{N,\downarrow}^\dagger\ldots c_{2N-2,\downarrow}^\dagger|0\rangle \\ &\quad+\frac{1}{\sqrt{\mathcal{N}}}\left\{\sum_{k=N/2}^{1}(-)^{k+1}g_k\sum_{i_{\frac{N}{2}-k}>\cdots>i_1=1}^{N-1}\hat{S}_{i_1}^+\ldots\hat{S}_{i_{\frac{N}{2}-k}}^+\right. \\ &\quad\times\left.\sum_{j_{\frac{N}{2}-k}>\cdots>j_1=N}^{2N-2}\hat{S}_{j_1}^-\ldots\hat{S}_{j_{\frac{N}{2}-k}}^-\right\}c_{1,\downarrow}^\dagger\ldots c_{N-1,\downarrow}^\dagger c_{N,\uparrow}^\dagger\ldots c_{2N-2,\uparrow}^\dagger|0\rangle\end{aligned} \tag{17}$$

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

$$\mathcal{N} = 2\sum_{k=1}^{N/2} g_k^2 \begin{pmatrix} N-1 \\ N/2-k \end{pmatrix}^2 \tag{18}$$

and the $g_k$ are given by

$$g_k = \frac{\begin{pmatrix} N/2+k-1 \\ N/2-1\end{pmatrix}}{\begin{pmatrix} N/2 \\ N/2-k\end{pmatrix}}. \tag{19}$$

Let

$$c_{\boldsymbol{k}} = \frac{1}{N}\sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} c_{\boldsymbol{r}}, \qquad d_{\boldsymbol{k}} = \frac{1}{N}\sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} d_{\boldsymbol{r}} \tag{20}$$

be the Fourier-transformed operators of the site annihilation operators $c_{\boldsymbol{r}}$ and $d_{\boldsymbol{r}}$ respectively. From equation (13) we obtain

$$c_{\boldsymbol{k}\downarrow} = d_{\boldsymbol{k}\downarrow}, \qquad c_{\boldsymbol{k}\uparrow} = d_{\boldsymbol{Q}-\boldsymbol{k}\uparrow}^\dagger, \qquad \boldsymbol{Q} = (\pi,\pi). \tag{21}$$

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

$$|\Sigma\rangle = |\Sigma_\uparrow\rangle \otimes |\Sigma_\downarrow\rangle, \qquad |\Sigma_\sigma\rangle = \prod_{\epsilon(\boldsymbol{k})<0} c_{\boldsymbol{k}\sigma}^\dagger|0\rangle. \tag{22}$$

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

$$|\Sigma_\downarrow\rangle = \prod_{\epsilon(\boldsymbol{k})<0} c_{\boldsymbol{k}\downarrow}^\dagger|0\rangle = \prod_{\epsilon(\boldsymbol{k})<0} d_{\boldsymbol{k}\downarrow}^\dagger|0\rangle \equiv |\tilde{\Sigma}_\downarrow\rangle \tag{23}$$

$$|\Sigma_\uparrow\rangle = \prod_{\epsilon(\boldsymbol{k})<0} c_{\boldsymbol{k}\uparrow}^\dagger|0\rangle = \prod_{\epsilon(\boldsymbol{k})<0} d_{\boldsymbol{Q}-\boldsymbol{k}\uparrow}\prod_{\boldsymbol{k}} d_{\boldsymbol{k}\uparrow}^\dagger|0\rangle. \tag{24}$$

Let $d_i$ be the operator obtained substituting $c_{\boldsymbol{k}}$ with $d_{\boldsymbol{k}}$ in the definition of $c_i$. We note that $\epsilon(\boldsymbol{k}) < 0$ corresponds to $\epsilon(\boldsymbol{Q}-\boldsymbol{k}) > 0$. Then, the spin-up filled-shell state $|\Sigma_\uparrow\rangle$ can be written as

$$\begin{aligned}|\Sigma_\uparrow\rangle = \prod_{\epsilon(\boldsymbol{k})\leqslant 0} d^\dagger_{\boldsymbol{k}\uparrow}|0\rangle = d^\dagger_{1,\uparrow}\ldots d^\dagger_{N-1,\uparrow}d^\dagger_{N,\uparrow}\ldots d^\dagger_{2N-2,\uparrow}\\ \prod_{\epsilon(\boldsymbol{k})<0} d^\dagger_{\boldsymbol{k}\uparrow}|0\rangle \equiv d^\dagger_{1,\uparrow}\ldots d^\dagger_{N-1,\uparrow}d^\dagger_{N,\uparrow}\ldots d^\dagger_{2N-2,\uparrow}|\tilde{\Sigma}_\uparrow\rangle\end{aligned} \tag{25}$$

and hence

$$|\Sigma_\uparrow\rangle\otimes|\Sigma_\downarrow\rangle = d^\dagger_{1,\uparrow}\ldots d^\dagger_{N-1,\uparrow}d^\dagger_{N,\uparrow}\ldots d^\dagger_{2N-2,\uparrow}|\tilde{\Sigma}_\uparrow\rangle\otimes|\tilde{\Sigma}_\downarrow\rangle. \tag{26}$$

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

$$c_{i\downarrow} = d_{i\downarrow}\quad \forall i, \qquad c_{i\uparrow} = \begin{cases} d^\dagger_{i\uparrow} & i = 1,\ldots,N-1\\ -d^\dagger_{i\uparrow} & i = N,\ldots,2N-2.\end{cases} \tag{27}$$

The above result implies that the raising operators $\hat{S}^+_i$ in the $d$ picture are given by

$$\hat{S}^+_i = \begin{cases} d_{i\uparrow}d_{i\downarrow} \equiv D_i & i = 1,\ldots,N-1\\ -d_{i\uparrow}d_{i\downarrow} \equiv -D_i & i = N,\ldots,2N-2.\end{cases} \tag{28}$$

These last three equations allow us to rewrite the whole ground state $|\Psi^{[0]}_{AF}\rangle = |\Phi^{[0]}_{AF}\rangle\otimes|\Sigma\rangle$ in the new picture:

$$\begin{aligned}
|\Psi^{[0]}_{AF}\rangle = {}& \frac{1}{\sqrt{\mathcal{N}}}\left\{\sum_{k=N/2}^{1} g_k \sum_{i_{\frac{N}{2}-k}>\cdots>i_1=1}^{N-1} D^\dagger_{i_1}\ldots D^\dagger_{i_{\frac{N}{2}-k}} \sum_{j_{\frac{N}{2}-k}>\cdots>j_1=N}^{2N-2} D_{j_1}\ldots D_{j_{\frac{N}{2}-k}}\right\}\\
&\times d_{1,\uparrow}\ldots d_{N-1,\uparrow}d^\dagger_{N,\downarrow}\ldots d^\dagger_{2N-2,\downarrow}d^\dagger_{1,\uparrow}\ldots d^\dagger_{N-1,\uparrow}d^\dagger_{N,\uparrow}\ldots d^\dagger_{2N-2,\uparrow}|\tilde{\Sigma}_\uparrow\rangle\otimes|\tilde{\Sigma}_\downarrow\rangle\\
&+\frac{1}{\sqrt{\mathcal{N}}}\left\{\sum_{k=N/2}^{1} g_k \sum_{i_{\frac{N}{2}-k}>\cdots>i_1=1}^{N-1} D_{i_1}\ldots D_{i_{\frac{N}{2}-k}} \sum_{j_{\frac{N}{2}-k}>\cdots>j_1=N}^{2N-2} D^\dagger_{j_1}\ldots D^\dagger_{j_{\frac{N}{2}-k}}\right\}\\
&\times d^\dagger_{1,\downarrow}\ldots d^\dagger_{N-1,\downarrow}d_{N,\uparrow}\ldots d_{2N-2,\uparrow}d^\dagger_{1,\uparrow}\ldots d^\dagger_{N-1,\uparrow}d^\dagger_{N,\uparrow}\ldots d^\dagger_{2N-2,\uparrow}|\tilde{\Sigma}_\uparrow\rangle\otimes|\tilde{\Sigma}_\downarrow\rangle\\
={}& \frac{1}{\sqrt{\mathcal{N}}}\left\{\sum_{k=N/2}^{1} g_k \sum_{i_{\frac{N}{2}-k}>\cdots>i_1=1}^{N-1}\ \sum_{j_{\frac{N}{2}-k}>\cdots>j_1=N}^{2N-2} D^\dagger_{i_1}\ldots D^\dagger_{i_{\frac{N}{2}-k}} D_{j_1}\ldots D_{j_{\frac{N}{2}-k}}\right\}\\
&\times d^\dagger_{N,\uparrow}\ldots d^\dagger_{2N-2,\uparrow}d^\dagger_{N,\downarrow}\ldots d^\dagger_{2N-2,\downarrow}|\tilde{\Sigma}_\uparrow\rangle\otimes|\tilde{\Sigma}_\downarrow\rangle\\
&+\frac{1}{\sqrt{\mathcal{N}}}\left\{\sum_{k=N/2}^{1} g_k \sum_{i_{\frac{N}{2}-k}>\cdots>i_1=1}^{N-1}\ \sum_{j_{\frac{N}{2}-k}>\cdots>j_1=N}^{2N-2} D_{i_1}\ldots D_{i_{\frac{N}{2}-k}} D^\dagger_{j_1}\ldots D^\dagger_{j_{\frac{N}{2}-k}}\right\}\\
&\times d^\dagger_{1,\uparrow}\ldots d^\dagger_{N-1,\uparrow}d^\dagger_{1,\downarrow}\ldots d^\dagger_{N-1,\downarrow}|\tilde{\Sigma}_\uparrow\rangle\otimes|\tilde{\Sigma}_\downarrow\rangle.
\end{aligned} \tag{29}$$

Therefore, the singlet ground state has the following form:

$$|\Psi^{[0]}_{AF}\rangle = \sum_\Gamma w_\Gamma \mathcal{D}^\dagger_{\Gamma\uparrow}|\tilde{\Sigma}_\uparrow\rangle\otimes\mathcal{D}^\dagger_{\Gamma\downarrow}|\tilde{\Sigma}_\downarrow\rangle, \tag{30}$$

where $\Gamma = \{\gamma_1,\ldots,\gamma_{N-1}\}$ with $1\leqslant\gamma_1<\cdots<\gamma_{N-1}\leqslant 2N-2$ and $\mathcal{D}^\dagger_\Gamma = d^\dagger_{\gamma_1}\ldots d^\dagger_{\gamma_{N-1}}$. $w_\Gamma$ 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 $w_\Gamma$ is given by

$$w_\Gamma = \frac{1}{\sqrt{\mathcal{N}}}g_{N/2-p}. \tag{31}$$

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

## 4. The spin correlation function

In this section we shall 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

$$G_{\rm spin}(\boldsymbol{r}) = \langle \Psi_{AF}^{[0]} | \boldsymbol{S}_{\boldsymbol{r}} \cdot \boldsymbol{S}_0 | \Psi_{AF}^{[0]} \rangle, \qquad \boldsymbol{S}_0 \equiv \boldsymbol{S}_{\boldsymbol{r}=(0,0)} \tag{32}$$

where $\boldsymbol{S}_{\boldsymbol{r}} = (\hat{S}^x_{\boldsymbol{r}}, \hat{S}^y_{\boldsymbol{r}}, \hat{S}^z_{\boldsymbol{r}})$ is the spin vector operator at site $\boldsymbol{r}$ with components

$$\hat{S}^x_{\boldsymbol{r}} = \tfrac{1}{2}(\hat{S}^+_{\boldsymbol{r}} + \hat{S}^-_{\boldsymbol{r}}), \qquad \hat{S}^y_{\boldsymbol{r}} = \frac{1}{2\mathrm{i}}(\hat{S}^+_{\boldsymbol{r}} - \hat{S}^-_{\boldsymbol{r}}), \qquad \hat{S}^z_{\boldsymbol{r}} = \tfrac{1}{2}(\hat{n}_{\boldsymbol{r}\uparrow} - \hat{n}_{\boldsymbol{r}\downarrow}) \tag{33}$$

and

$$\hat{S}^+_{\boldsymbol{r}} = c^\dagger_{\boldsymbol{r}\uparrow} c_{\boldsymbol{r}\downarrow}, \qquad \hat{S}^-_{\boldsymbol{r}} = (\hat{S}^+_{\boldsymbol{r}})^\dagger = c^\dagger_{\boldsymbol{r}\downarrow} c_{\boldsymbol{r}\uparrow}. \tag{34}$$

Taking into account that $\Psi_{AF}^{[0]}$ is a singlet, one has $\langle \hat{S}^x_{\boldsymbol{r}} \hat{S}^x_0 \rangle = \langle \hat{S}^y_{\boldsymbol{r}} \hat{S}^y_0 \rangle = \langle \hat{S}^z_{\boldsymbol{r}} \hat{S}^z_0 \rangle$ and hence

$$G_{\rm spin}(\boldsymbol{r}) = \tfrac{3}{4}[\langle \hat{S}^-_{\boldsymbol{r}} \hat{S}^+_0 + \hat{S}^+_{\boldsymbol{r}} \hat{S}^-_0 \rangle] \tag{35}$$

with $\hat{S}^\pm_0 = \hat{S}^\pm_{\boldsymbol{r}=(0,0)}$ and $\langle \ldots \rangle$ means the expectation value over the ground state $|\Psi_{AF}^{[0]}\rangle$. Since $|\Psi_{AF}^{[0]}\rangle$ is a real linear combination of real basis vectors, $G^{-+}(\boldsymbol{r}) \equiv \langle \hat{S}^-_{\boldsymbol{r}} \hat{S}^+_0 \rangle \in \Re \;\; \forall \boldsymbol{r}$ and this implies

$$G^{-+}(\boldsymbol{r}) = G^{-+}(\boldsymbol{r})^* = \langle \hat{S}^-_0 \hat{S}^+_{\boldsymbol{r}} \rangle = \langle \hat{S}^+_{\boldsymbol{r}} \hat{S}^-_0 \rangle - 2\delta_{\boldsymbol{r},0} \langle \hat{S}^z_{\boldsymbol{r}} \rangle. \tag{36}$$

Noting that $|\Psi_{AF}^{[0]}\rangle$ is a translation-invariant state, $\langle \hat{S}^z_0 \rangle = \frac{1}{N^2} \sum_{\boldsymbol{r}} \langle \hat{S}^z_{\boldsymbol{r}} \rangle = \frac{1}{N^2} \langle \hat{S}^z \rangle = 0$ and hence

$$G^{-+}(\boldsymbol{r}) = \langle \hat{S}^+_{\boldsymbol{r}} \hat{S}^-_0 \rangle \equiv G^{+-}(\boldsymbol{r}). \tag{37}$$

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

$$G_{\rm spin}(\boldsymbol{r}) = \tfrac{3}{2} G^{-+}(\boldsymbol{r}), \tag{38}$$

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

$$\begin{aligned} G^{-+}(\boldsymbol{r}) &= \langle c^\dagger_{\boldsymbol{r}\downarrow} c_{\boldsymbol{r}\uparrow} c^\dagger_{0\uparrow} c_{0\downarrow} \rangle = (-)^{x+y} \langle d^\dagger_{\boldsymbol{r}\downarrow} d^\dagger_{\boldsymbol{r}\uparrow} d_{0\uparrow} d_{0\downarrow} \rangle \\ &= (-)^{x+y} \sum_{\Gamma_1 \Gamma_2} w_{\Gamma_1} w_{\Gamma_2} \langle \tilde{\Sigma}_\downarrow | \mathcal{D}_{\Gamma_1\downarrow} d^\dagger_{\boldsymbol{r}\downarrow} d_{0\downarrow} \mathcal{D}^\dagger_{\Gamma_2\downarrow} | \tilde{\Sigma}_\downarrow \rangle \\ &\quad \times \langle \tilde{\Sigma}_\uparrow | \mathcal{D}_{\Gamma_1\uparrow} d^\dagger_{\boldsymbol{r}\uparrow} d_{0\uparrow} \mathcal{D}^\dagger_{\Gamma_2\uparrow} | \tilde{\Sigma}_\uparrow \rangle \equiv (-)^{x+y} \sum_{\Gamma_1 \Gamma_2} w_{\Gamma_1} w_{\Gamma_2} G_{\Gamma_1 \Gamma_2}(\boldsymbol{r})^2, \end{aligned} \tag{39}$$

where, dropping the spin index,

$$G_{\Gamma_1 \Gamma_2}(\boldsymbol{r}) = \langle \Gamma_1 | d^\dagger_{\boldsymbol{r}} d_0 | \Gamma_2 \rangle, \qquad |\Gamma\rangle = \mathcal{D}^\dagger_\Gamma |\tilde{\Sigma}\rangle. \tag{40}$$

Here and in the following $c_{0\sigma} \equiv c_{\boldsymbol{r}=(0,0)\sigma}$ and $d_{0\sigma} \equiv d_{\boldsymbol{r}=(0,0)\sigma}$. Since the $w_\Gamma$ are non-negative, equation (39) shows that $G^{-+}(\boldsymbol{r})$ is positive if $\boldsymbol{r}$ belongs to the sublattice $\mathcal{A}$ containing

$\boldsymbol{r} = (0,0)$ and negative otherwise. This was pointed out in [17]. All the information on the spin correlation function is enclosed in the site-dependent matrix elements $G_{\Gamma_1\Gamma_2}(\boldsymbol{r})$. To evaluate them we write the annihilation operator $d_{\boldsymbol{r}}$ as the sum of three pieces

$$\begin{aligned} d_{\boldsymbol{r}} &= \frac{1}{N}\sum_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} d_{\boldsymbol{k}} = \frac{\sqrt{|\mathcal{S}_{hf}|}}{N} d_1(\boldsymbol{r}) + \frac{\sqrt{|\mathcal{S}|}}{N} d_\xi(\boldsymbol{r}) + \frac{\sqrt{|\mathcal{S}|}}{N} d_{\bar{\xi}}(\boldsymbol{r}) \\ &\equiv \rho_{hf} d_1(\boldsymbol{r}) + \rho[d_\xi(\boldsymbol{r}) + d_{\bar{\xi}}(\boldsymbol{r})], \end{aligned} \tag{41}$$

with

$$\begin{aligned} d_1(\boldsymbol{r}) &= \frac{1}{\sqrt{|\mathcal{S}_{hf}|}} \sum_{\epsilon(\boldsymbol{k})=0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} d_{\boldsymbol{k}}, \qquad d_\xi(\boldsymbol{r}) = \frac{1}{\sqrt{|\mathcal{S}|}} \sum_{\epsilon(\boldsymbol{k})<0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} d_{\boldsymbol{k}}, \\ d_{\bar{\xi}}(\boldsymbol{r}) &= \frac{1}{\sqrt{|\mathcal{S}|}} \sum_{\epsilon(\boldsymbol{k})>0} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} d_{\boldsymbol{k}} \end{aligned} \tag{42}$$

and $|\mathcal{S}_{hf}| = 2N-2$, $|\mathcal{S}| = \frac{1}{2}(N^2 - |\mathcal{S}_{hf}|)$. We observe that $d_1(0) = d_1(\boldsymbol{r} = (0,0))$ belongs to $\mathrm{A}_1$ and that it can be written as a real linear combination of all the $\mathrm{A}_1$-symmetric annihilation operators of the local basis. By a unitary transformation on this $\mathrm{A}_1$ subspace we may arrange that $d_1(0)$ is the new $d_1$. Thus, from now on, the one-body local basis $\{d_i^\dagger|0\rangle,\ i = 1,\ldots,2N-2\}$, is such that the set of the $\mathrm{A}_1$-symmetric local states contains $d_1^\dagger(0)|0\rangle$ and $d_1^\dagger|0\rangle = d_1^\dagger(0)|0\rangle$.

Taking equation (41) into account one can express $G_{\Gamma_1\Gamma_2}(\boldsymbol{r})$ as the sum of two terms:

$$G_{\Gamma_1\Gamma_2}(\boldsymbol{r}) = \rho_{hf}^2\langle\Gamma_1|d_1^\dagger(\boldsymbol{r})d_1|\Gamma_2\rangle + \rho^2\langle\Gamma_1|d_\xi^\dagger(\boldsymbol{r})d_\xi|\Gamma_2\rangle \equiv \rho_{hf}^2 G_{\Gamma_1\Gamma_2}^{[hf]}(\boldsymbol{r}) + \rho^2 G_{\Gamma_1\Gamma_2}^{[\xi]}(\boldsymbol{r}), \tag{43}$$

with $d_1 \equiv d_1(0)$ and $d_\xi \equiv d_\xi(0) \equiv d_\xi(\boldsymbol{r} = (0,0))$. $G_{\Gamma_1\Gamma_2}^{[\xi]}(\boldsymbol{r})$ can be easily evaluated:

$$\begin{aligned} G_{\Gamma_1\Gamma_2}^{[\xi]}(\boldsymbol{r}) &= \langle\Gamma_1|d_\xi^\dagger(\boldsymbol{r})d_\xi|\Gamma_2\rangle \\ &= \delta_{\Gamma_1\Gamma_2}\sum_{\epsilon(\boldsymbol{k}_1)<0}\sum_{\epsilon(\boldsymbol{k}_2)<0} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{r}}\frac{1}{|\mathcal{S}|}\langle\tilde{\Sigma}|d_{\boldsymbol{k}_1}^\dagger d_{\boldsymbol{k}_2}|\tilde{\Sigma}\rangle = \delta_{\Gamma_1\Gamma_2}\frac{\mathcal{T}(\boldsymbol{r})}{|\mathcal{S}|} \end{aligned} \tag{44}$$

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

$$\begin{aligned} G^{-+}(\boldsymbol{r}) = (-)^{x+y}\Bigg\{&\rho_{hf}^4\sum_{\Gamma_1\Gamma_2} w_{\Gamma_1}w_{\Gamma_2}G_{\Gamma_1\Gamma_2}^{[hf]}(\boldsymbol{r})^2 + 2\rho^2\rho_{hf}^2\frac{\mathcal{T}(\boldsymbol{r})}{|\mathcal{S}|} \\ &\times\sum_{\Gamma} w_\Gamma^2 G_{\Gamma\Gamma}^{[hf]}(\boldsymbol{r}) + \rho^4\frac{\mathcal{T}(\boldsymbol{r})^2}{|\mathcal{S}|^2}\sum_{\Gamma} w_\Gamma^2\Bigg\}. \end{aligned} \tag{45}$$

By definition $\sum_\Gamma w_\Gamma^2 = \langle\Psi_{AF}^{[0]}|\Psi_{AF}^{[0]}\rangle = 1$. To evaluate the diagonal matrix elements $G_{\Gamma\Gamma}^{[hf]}(\boldsymbol{r})$ 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 $d_1(\boldsymbol{r})$ can be expanded as

$$d_1(\boldsymbol{r}) = \begin{cases} \displaystyle\sum_{i=1}^{N-1} t_i(\boldsymbol{r})d_i, & t_i(\boldsymbol{r}) \in \Re \quad x+y \text{ even} \\ \displaystyle\sum_{i=N}^{2N-2} t_i(\boldsymbol{r})d_i, & t_i(\boldsymbol{r}) \in \Re \quad x+y \text{ odd} \end{cases} \tag{46}$$

and $G^{[hf]}_{\Gamma\Gamma}(\boldsymbol{r})$ becomes

$$G^{[hf]}_{\Gamma\Gamma}(\boldsymbol{r}) = \langle\Gamma|d_1^\dagger(\boldsymbol{r})d_1|\Gamma\rangle = \begin{cases} t_1(\boldsymbol{r})\delta_{1\gamma_1} & x+y \text{ even} \\ 0 & x+y \text{ odd} \end{cases} \tag{47}$$

where $\gamma_1$ is the first index of the configuration $\Gamma$ (we recall that $\Gamma = \{\gamma_1, \ldots, \gamma_{N-1}\}$ with $1 \leqslant \gamma_1 < \cdots < \gamma_{N-1} \leqslant 2N-2$). Substituting this result into equation (45) we see we need to evaluate $\sum_\Gamma w_\Gamma^2 \delta_{1\gamma_1}$. This can be done by observing that $|\Phi^{[0]}_{AF}\rangle$ can be rewritten in the $c$ picture as

$$|\Phi^{[0]}_{AF}\rangle = |\Phi^{[0]}_{\uparrow}\rangle - |\Phi^{[0]}_{\downarrow}\rangle \tag{48}$$

with

$$|\Phi^{[0]}_{\uparrow}\rangle = \frac{1}{\sqrt{\mathcal{N}}}\sum_{k=0}^{N-2}(-)^k f_k \sum_{i_k>\cdots>i_1=2}^{N-1}\ \sum_{j_k>\cdots>j_1=N}^{2N-2} \times \hat{S}^-_{i_k}\ldots\hat{S}^-_{i_1}\hat{S}^+_{j_k}\ldots\hat{S}^+_{j_1}c^\dagger_{1,\uparrow}\ldots c^\dagger_{N-1,\uparrow}c^\dagger_{N,\downarrow}\ldots c^\dagger_{2N-2,\downarrow}|0\rangle \tag{49}$$

$$|\Phi^{[0]}_{\downarrow}\rangle = \frac{1}{\sqrt{\mathcal{N}}}\sum_{k=0}^{N-2}(-)^k f_k \sum_{i_k>\cdots>i_1=2}^{N-1}\ \sum_{j_k>\cdots>j_1=N}^{2N-2} \times \hat{S}^+_{i_k}\ldots\hat{S}^+_{i_1}\hat{S}^-_{j_k}\ldots\hat{S}^-_{j_1}c^\dagger_{1,\downarrow}\ldots c^\dagger_{N-1,\downarrow}c^\dagger_{N,\uparrow}\ldots c^\dagger_{2N-2,\uparrow}|0\rangle \tag{50}$$

and

$$f_k = \begin{cases} g_{N/2-k} & k = 0, \ldots, N/2-1 \\ g_{k+1-N/2} & k = N/2, \ldots, N-1. \end{cases} \tag{51}$$

All the configurations contained in $|\Phi^{[0]}_{\downarrow}\rangle$ are such that in the particle–hole transformed picture $\delta_{1\gamma_1} = 1$. On the other hand, all the configurations contained in $|\Phi^{[0]}_{\uparrow}\rangle$ are such that in the particle–hole transformed picture $\delta_{1\gamma_1} = 0$. Therefore

$$\sum_\Gamma w_\Gamma^2 \delta_{1\gamma_1} = \langle\Phi^{[0]}_{\downarrow}|\Phi^{[0]}_{\downarrow}\rangle = \langle\Phi^{[0]}_{\uparrow}|\Phi^{[0]}_{\uparrow}\rangle = \tfrac{1}{2}. \tag{52}$$

The second term in equation (45) is totally determined once we know $t_1(\boldsymbol{r})$. By definition

$$t_1(\boldsymbol{r}) = \langle 0|d_1^\dagger(\boldsymbol{r})d_1|0\rangle = \frac{\mathcal{T}_{hf}(\boldsymbol{r})}{|\mathcal{S}_{hf}|}, \tag{53}$$

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

$$G^{-+}(\boldsymbol{r}) = (-)^{x+y}\left\{\rho_{hf}^4 \sum_{\Gamma_1\Gamma_2} w_{\Gamma_1}w_{\Gamma_2}G^{[hf]}_{\Gamma_1\Gamma_2}(\boldsymbol{r})^2 + \frac{1}{N^4}\mathcal{T}(\boldsymbol{r})[\mathcal{T}(\boldsymbol{r}) + \mathcal{T}_{hf}(\boldsymbol{r})]\right\} \tag{54}$$

where we have used equations (47), (52) and (53).

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

$$\begin{aligned}(-)^{x+y}\sum_{\Gamma_1\Gamma_2} w_{\Gamma_1}w_{\Gamma_2}G^{[hf]}_{\Gamma_1\Gamma_2}(\boldsymbol{r})^2 &= \langle\Psi^{[0]}_{AF}|c^\dagger_{1,\downarrow}c_{1,\uparrow}\hat{T}(\boldsymbol{r})c^\dagger_{1,\uparrow}c_{1,\downarrow}|\Psi^{[0]}_{AF}\rangle \\ &= \langle\Phi^{[0]}_{\downarrow}|c^\dagger_{1,\downarrow}c_{1,\uparrow}\hat{T}(\boldsymbol{r})c^\dagger_{1,\uparrow}c_{1,\downarrow}|\Phi^{[0]}_{\downarrow}\rangle \equiv X(\boldsymbol{r})\end{aligned} \tag{55}$$

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

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

$$\boxed{X(\boldsymbol{r}) = \frac{(-)^{x+y}}{|\mathcal{S}_{hf}|^2}\begin{cases} A + B \times \mathcal{T}_{hf}^2(\boldsymbol{r}) & x+y \text{ even} \\ A + B \times (4N-4) & x+y \text{ odd}\end{cases}} \tag{56}$$

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

$$\boxed{G_{\text{spin}}(\boldsymbol{r}) = \frac{3}{2}\frac{(-)^{x+y}}{N^4}\left[\mathcal{T}(\boldsymbol{r})[\mathcal{T}(\boldsymbol{r}) + \mathcal{T}_{hf}(\boldsymbol{r})] + \begin{cases} A + B \times \mathcal{T}_{hf}^2(\boldsymbol{r}) & x+y \text{ even} \\ A + B \times (4N-4) & x+y \text{ odd}\end{cases}\right].} \tag{57}$$

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

$$\sum_{\boldsymbol{r}} G_{\text{spin}}(\boldsymbol{r}) = 0 \tag{58}$$

holds. Indeed, let us consider the identities

$$\sum_{\boldsymbol{r}}(-1)^{x+y}\mathcal{T}(\boldsymbol{r})^2 = \sum_{\boldsymbol{r}}\sum_{\epsilon(\boldsymbol{k}),\epsilon(\boldsymbol{k}')<0}(-1)^{x+y}\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}+\boldsymbol{k}')\cdot\boldsymbol{r}} = \sum_{\epsilon(\boldsymbol{k}),\epsilon(\boldsymbol{k}')<0}\sum_{\boldsymbol{r}}\mathrm{e}^{-\mathrm{i}(\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{Q})\cdot\boldsymbol{r}}; \tag{59}$$

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

$$\sum_{\boldsymbol{r}}(-1)^{x+y}\mathcal{T}(\boldsymbol{r})^2 = 0, \tag{60}$$

and, similarly,

$$\sum_{\boldsymbol{r}}(-1)^{x+y}\mathcal{T}(\boldsymbol{r})\mathcal{T}_{hf}(\boldsymbol{r}) = 0. \tag{61}$$

On the other hand, since

$$\sum_{\boldsymbol{r}\in\mathcal{A}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{N^2}{2}(\delta_{\boldsymbol{k},0} + \delta_{\boldsymbol{k},\boldsymbol{Q}}), \tag{62}$$

where $\mathcal{A}$ is the sublattice with sites having $x+y$ even, one obtains

$$\sum_{\boldsymbol{r}\in\mathcal{A}}\mathcal{T}_{hf}(\boldsymbol{r})^2 = \frac{N^2}{2}(4N-4) \tag{63}$$

and hence equation (58).

## 5. The charge correlation function

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

$$G_{\text{charge}}(\boldsymbol{r}) \equiv \langle \Psi_{AF}^{[0]} | \hat{n}_{\boldsymbol{r}}^{[+]} \hat{n}_0^{[+]} | \Psi_{AF}^{[0]} \rangle, \tag{64}$$

while the spin correlation function can be written as

$$G_{\text{spin}}(\boldsymbol{r}) = 3\langle \Psi_{AF}^{[0]} | \hat{S}_{\boldsymbol{r}}^z \hat{S}_0^z | \Psi_{AF}^{[0]} \rangle = \tfrac{3}{4} \langle \Psi_{AF}^{[0]} | \hat{n}_{\boldsymbol{r}}^{[-]} \hat{n}_0^{[-]} | \Psi_{AF}^{[0]} \rangle, \tag{65}$$

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

$$|\Psi_{AF}^{[0]}\rangle = |\Psi_{\uparrow}^{[0]}\rangle - |\Psi_{\downarrow}^{[0]}\rangle, \tag{66}$$

with $|\Psi_{\sigma}^{[0]}\rangle = |\Phi_{\sigma}^{[0]}\rangle \otimes |\Sigma\rangle$, be a suitable decomposition of the singlet ground-state wavefunction (see equation (48)). Exploiting the invariance of $\langle \Psi_{\sigma}^{[0]} | \hat{n}_{\boldsymbol{r}}^{[\pm]} \hat{n}_0^{[\pm]} | \Psi_{\sigma'}^{[0]} \rangle$ for simultaneous flips of $\sigma$ and $\sigma'$ we obtain

$$G_{\text{charge}}(\boldsymbol{r}) = 2[\langle \Psi_{\uparrow}^{[0]} | \hat{n}_0^{[+]} \hat{T}(\boldsymbol{r}) \hat{n}_0^{[+]} | \Psi_{\uparrow}^{[0]} \rangle - \langle \Psi_{\downarrow}^{[0]} | \hat{n}_0^{[+]} \hat{T}(\boldsymbol{r}) \hat{n}_0^{[+]} | \Psi_{\uparrow}^{[0]} \rangle] \tag{67}$$

$$G_{\text{spin}}(\boldsymbol{r}) = \tfrac{3}{2}[\langle \Psi_{\uparrow}^{[0]} | \hat{n}_0^{[-]} \hat{T}(\boldsymbol{r}) \hat{n}_0^{[-]} | \Psi_{\uparrow}^{[0]} \rangle - \langle \Psi_{\downarrow}^{[0]} | \hat{n}_0^{[-]} \hat{T}(\boldsymbol{r}) \hat{n}_0^{[-]} | \Psi_{\uparrow}^{[0]} \rangle], \tag{68}$$

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

$$\hat{n}_{\boldsymbol{r}\sigma} = \hat{T}^{\dagger}(\boldsymbol{r}) \hat{n}_{0\sigma} \hat{T}(\boldsymbol{r}) \tag{69}$$

and $\hat{T}(\boldsymbol{r})|\Psi_{AF}^{[0]}\rangle = |\Psi_{AF}^{[0]}\rangle$ has been used. The action of $\hat{n}_0^{[\pm]}$ on the state $|\Psi_{\sigma}^{[0]}\rangle$ can be easily evaluated. We can express $c_{\boldsymbol{r}}$ as the sum of three operators as in equation (41)

$$c_{\boldsymbol{r}} = \rho_{hf} c_1(\boldsymbol{r}) + \rho[c_{\xi}(\boldsymbol{r}) + c_{\bar{\xi}}(\boldsymbol{r})] \tag{70}$$

where $c_1$, $c_{\xi}$ and $c_{\bar{\xi}}$ are defined as $d_1$, $d_{\xi}$ and $d_{\bar{\xi}}$ in equation (42), but $d_{\boldsymbol{k}}$ must be substituted with $c_{\boldsymbol{k}}$. Then we obtain

$$\begin{aligned} \hat{n}_0^{[\pm]} |\Psi_{\uparrow}^{[0]}\rangle &= (\hat{n}_{0\uparrow} \pm \hat{n}_{0\downarrow}) |\Psi_{\uparrow}^{[0]}\rangle = [(\rho_{hf}^2 + \rho^2 \pm \rho^2) \\ &\quad + \rho\rho_{hf}(c_{\bar{\xi}\uparrow}^{\dagger} c_{1,\uparrow} \pm c_{1,\downarrow}^{\dagger} c_{\xi\downarrow}) + \rho^2 (c_{\bar{\xi}\uparrow}^{\dagger} c_{\xi\uparrow} \pm c_{\bar{\xi}\downarrow}^{\dagger} c_{\xi\downarrow})] |\Psi_{\uparrow}^{[0]}\rangle, \end{aligned} \tag{71}$$

$$\begin{aligned} \hat{n}_0^{[\pm]} |\Psi_{\downarrow}^{[0]}\rangle &= (\hat{n}_{0\uparrow} \pm \hat{n}_{0\downarrow}) |\Psi_{\downarrow}^{[0]}\rangle = [(\rho^2 \pm \rho_{hf}^2 \pm \rho^2) \\ &\quad + \rho\rho_{hf}(c_{1,\uparrow}^{\dagger} c_{\xi\uparrow} \pm c_{\bar{\xi}\downarrow}^{\dagger} c_{1,\downarrow}) + \rho^2 (c_{\bar{\xi}\uparrow}^{\dagger} c_{\xi\uparrow} \pm c_{\bar{\xi}\downarrow}^{\dagger} c_{\xi\downarrow})] |\Psi_{\downarrow}^{[0]}\rangle. \end{aligned} \tag{72}$$

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

$$\begin{aligned} &\langle \Psi_{\uparrow}^{[0]} | \hat{n}_0^{[\pm]} \hat{T}(\boldsymbol{r}) \hat{n}_0^{[\pm]} | \Psi_{\uparrow}^{[0]} \rangle \\ &\quad = [(\rho_{hf}^2 + \rho^2 \pm \rho^2)^2 + 2\rho^4 \langle \Sigma | c_{\xi\uparrow}^{\dagger} c_{\bar{\xi}\uparrow} \hat{T}(\boldsymbol{r}) c_{\bar{\xi}\uparrow}^{\dagger} c_{\xi\uparrow} | \Sigma \rangle] \langle \Phi_{\uparrow}^{[0]} | \hat{T}(\boldsymbol{r}) | \Phi_{\uparrow}^{[0]} \rangle \\ &\quad + \rho^2 \rho_{hf}^2 (\langle \Phi_{\uparrow}^{[0]} | c_{1,\uparrow}^{\dagger} \hat{T}(\boldsymbol{r}) c_{1,\uparrow} | \Phi_{\uparrow}^{[0]} \rangle \langle \Sigma | c_{\bar{\xi}\uparrow} \hat{T}(\boldsymbol{r}) c_{\bar{\xi}\uparrow}^{\dagger} | \Sigma \rangle \\ &\quad + \langle \Phi_{\uparrow}^{[0]} | c_{1,\downarrow} \hat{T}(\boldsymbol{r}) c_{1,\downarrow}^{\dagger} | \Phi_{\uparrow}^{[0]} \rangle \langle \Sigma | c_{\xi\downarrow}^{\dagger} \hat{T}(\boldsymbol{r}) c_{\xi\downarrow} | \Sigma \rangle) \end{aligned} \tag{73}$$

and

$$\begin{aligned} &\langle \Psi_{\downarrow}^{[0]} | \hat{n}_0^{[\pm]} \hat{T}(\boldsymbol{r}) \hat{n}_0^{[\pm]} | \Psi_{\uparrow}^{[0]} \rangle \\ &\quad = [\pm(\rho_{hf}^2 + \rho^2 \pm \rho^2)^2 + 2\rho^4 \langle \Sigma | c_{\xi\uparrow}^{\dagger} c_{\bar{\xi}\uparrow} \hat{T}(\boldsymbol{r}) c_{\bar{\xi}\uparrow}^{\dagger} c_{\xi\uparrow} | \Sigma \rangle] \langle \Phi_{\downarrow}^{[0]} | \hat{T}(\boldsymbol{r}) | \Phi_{\uparrow}^{[0]} \rangle \end{aligned} \tag{74}$$

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

$$1 = \langle\Phi^{[0]}_{AF}|\hat{T}(\boldsymbol{r})|\Phi^{[0]}_{AF}\rangle = 2[\langle\Phi^{[0]}_{\uparrow}|\hat{T}(\boldsymbol{r})|\Phi^{[0]}_{\uparrow}\rangle - \langle\Phi^{[0]}_{\downarrow}|\hat{T}(\boldsymbol{r})||\Phi^{[0]}_{\uparrow}\rangle] \tag{75}$$

and hence

$$\boxed{\langle\Phi^{[0]}_{\downarrow}|\hat{T}(\boldsymbol{r})|\Phi^{[0]}_{\uparrow}\rangle = \langle\Phi^{[0]}_{\uparrow}|\hat{T}(\boldsymbol{r})|\Phi^{[0]}_{\uparrow}\rangle - \tfrac{1}{2}.} \tag{76}$$

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

$$\begin{aligned}
&\langle\Psi^{[0]}_{\uparrow}|\hat{n}^{[\pm]}_{0}\hat{T}(\boldsymbol{r})\hat{n}^{[\pm]}_{0}|\Psi^{[0]}_{\uparrow}\rangle - \langle\Psi^{[0]}_{\downarrow}|\hat{n}^{[\pm]}_{0}\hat{T}(\boldsymbol{r})\hat{n}^{[\pm]}_{0}|\Psi^{[0]}_{\uparrow}\rangle \\
&\quad= \pm\ \tfrac{1}{2}(\rho^2_{hf} + \rho^2 \pm \rho^2)^2 + \rho^4\langle\Sigma|c^{\dagger}_{\xi\uparrow}c_{\bar{\xi}\uparrow}\hat{T}(\boldsymbol{r})c^{\dagger}_{\bar{\xi}\uparrow}c_{\xi\uparrow}|\Sigma\rangle \\
&\qquad+ \rho^2\rho^2_{hf}[\langle\Phi^{[0]}_{\uparrow}|c^{\dagger}_{1,\uparrow}\hat{T}(\boldsymbol{r})c_{1,\uparrow}|\Phi^{[0]}_{\uparrow}\rangle\langle\Sigma|c_{\bar{\xi}\uparrow}\hat{T}(\boldsymbol{r})c^{\dagger}_{\bar{\xi}\uparrow}|\Sigma\rangle \\
&\qquad+ \langle\Phi^{[0]}_{\uparrow}|c_{1,\downarrow}\hat{T}(\boldsymbol{r})c^{\dagger}_{1,\downarrow}|\Phi^{[0]}_{\uparrow}\rangle\langle\Sigma|c^{\dagger}_{\xi\downarrow}\hat{T}(\boldsymbol{r})c_{\xi\downarrow}|\Sigma\rangle] \\
&\qquad+ [(1\pm(-1))(\rho^2_{hf} + \rho^2 \pm \rho^2)^2]\langle\Phi^{[0]}_{\uparrow}|\hat{T}(\boldsymbol{r})|\Phi^{[0]}_{\uparrow}\rangle
\end{aligned} \tag{77}$$

and so, since $\rho^2_{hf} + 2\rho^2 = 1$,

$$\boxed{G_{\text{charge}}(\boldsymbol{r}) = 1 + \tfrac{4}{3}G_{\text{spin}}(\boldsymbol{r}) + \rho^4_{hf}[1 - 4Y(\boldsymbol{r})],} \tag{78}$$

where

$$Y(\boldsymbol{r}) \equiv \langle\Phi^{[0]}_{\uparrow}|\hat{T}(\boldsymbol{r})|\Phi^{[0]}_{\uparrow}\rangle. \tag{79}$$

We postpone to appendix 6 the explicit calculation of $Y(\boldsymbol{r})$. Here we limit ourselves to presenting the final results

$$\boxed{Y(\boldsymbol{r}) = \frac{1}{4} + \frac{(-)^{x+y}}{|\mathcal{S}_{hf}|^2} \times \begin{cases} D + E \times \mathcal{T}_{hf}(\boldsymbol{r})^2 & x+y \text{ even} \\ D + E \times (4N-4) & x+y \text{ odd.}\end{cases}} \tag{80}$$

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

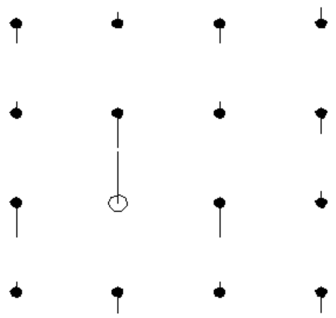
$$\sum_{\boldsymbol{r}} G_{\text{charge}}(\boldsymbol{r}) = N^2 \tag{81}$$

is satisfied.

## 6. 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 [5]). On 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 [5] and our result is identical to that reported there, which was obtained by second-order perturbation theory on the computer.

More data [18,19] on the $4\times 4$ cluster were obtained by Fano, Ortolani and Parola by exact diagonalization augmented by an intensive use of group theory techniques. On the right-hand side of figure 1 we report the spin correlation function in real space, $G_{\text{spin}}(\boldsymbol{r})$ in equation (57), along a triangular path. Although our results are almost exact for $U \to 0$, remarkably the



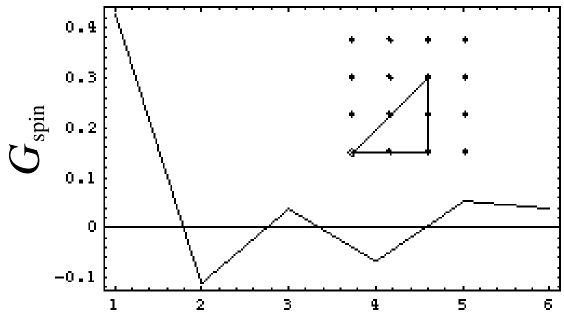



**Figure 1.** Left: the spin correlation function between the origin (empty circle) and the other sites; the length of the lines is proportional to the absolute value of the correlation function, and the sign is positive for the lines going up. The on-site value is reduced by a factor of 0.4 for graphical convenience. Right: the spin correlation function in real space for the 4 × 4 model, along a anticlockwise path from the origin (empty circle, see the inset).

trend is quite the same as the one reported in [18] for $U = 4$. An overall factor of four depends on the definition of the spin operators in [18], lacking the usual $1/2$ factor.

The analytic expression of the spin correlation function in equation (57) agrees 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 3 above.

The Fourier transform of the spin correlation function

$$G_{\text{spin}}(\boldsymbol{k}) \equiv \sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} G_{\text{spin}}(\boldsymbol{r}) \tag{82}$$

is shown in figure 3; the ticks on the $x$ axis correspond to the points $\Gamma \equiv (0, 0)$, $\mathrm{P} \equiv (\pi, 0)$, $\mathrm{Q} \equiv (\pi, \pi)$ 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.

The charge correlation function in real space shows characteristic structures with two intersecting channels at 45° from the axes as exemplified in figure 4 for the $10 \times 10$ 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.

The Fourier-transformed charge correlation function is dominated by a delta function at $\Gamma \equiv (0, 0)$ resulting from the almost constant distribution in real space. In figure 5 we have removed that delta. The figure represents $G_{\text{charge}}(\boldsymbol{k}) \equiv \sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} G_{\text{charge}}(\boldsymbol{r})$ along the path Γ, P, Q, Γ (see figure caption for details) for the $10 \times 10$ square lattice. Already at this cluster size $G_{\text{charge}}(\boldsymbol{k})$ 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 wavefunction $|\Psi_{AF}^{[0]}\rangle$ 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 $U \leqslant t/N^2$, 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-

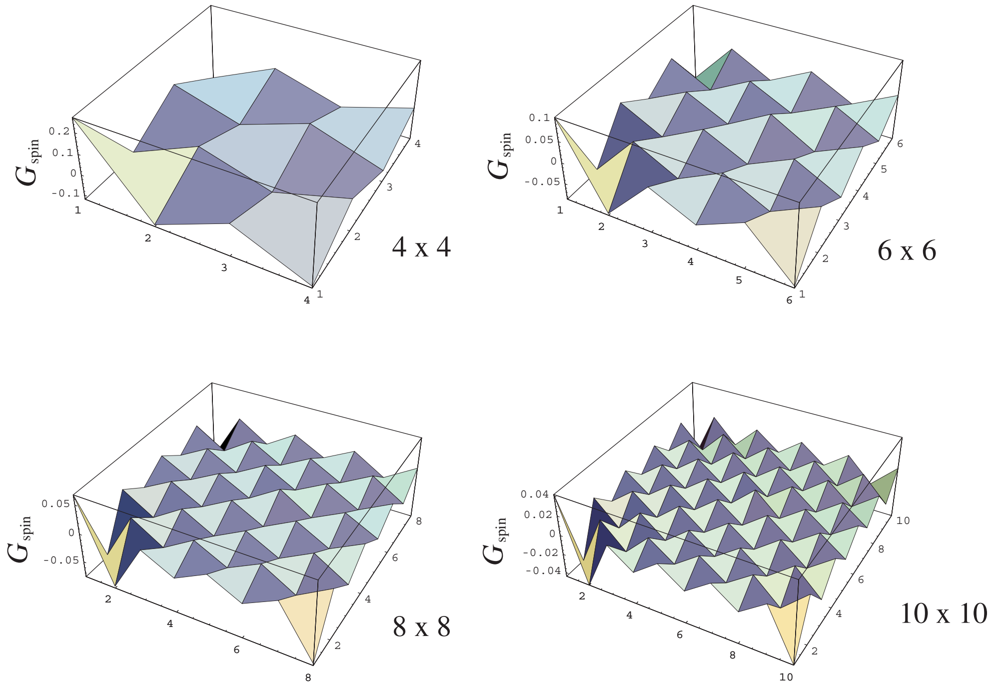



**Figure 2.** The spin correlation function in real space for the $4 \times 4$, $6 \times 6$, $8 \times 8$ and $10 \times 10$ clusters. The Shen–Qiu–Tian property is evident.

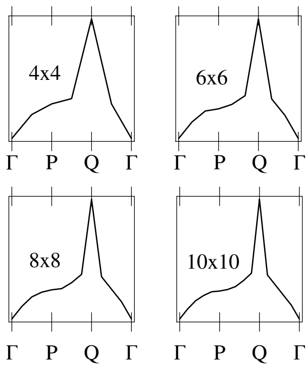



**Figure 3.** The Fourier transform of the spin correlation functions in clusters of various sizes. The ticks on the $x$ axis correspond to Γ, P, Q and Γ, as usual.

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 $\mathcal{S}_{hf}$; 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 [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.

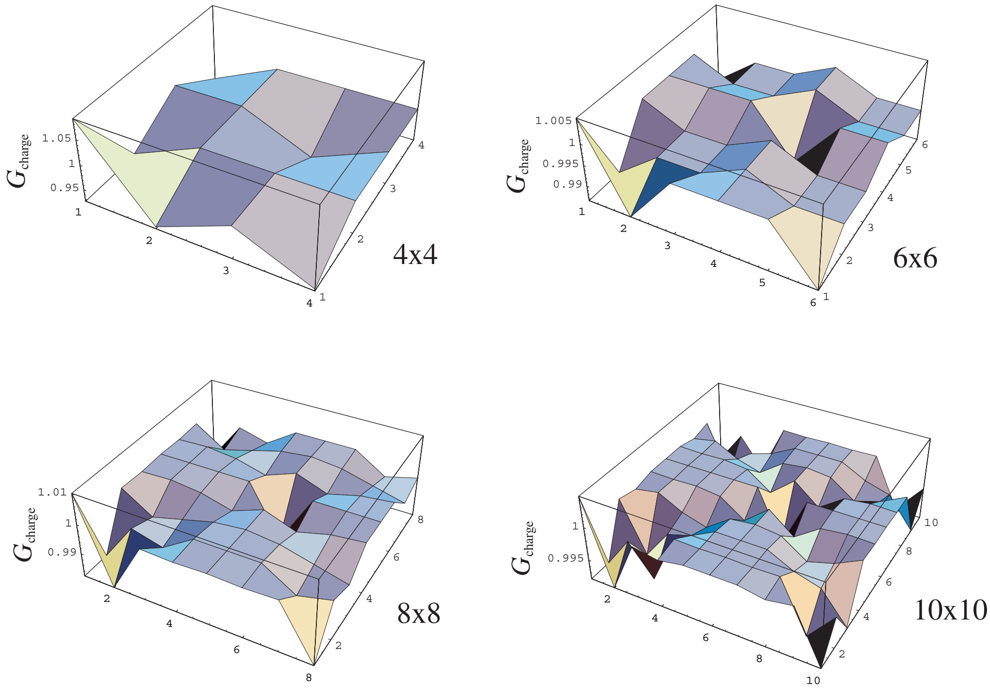



**Figure 4.** Real space representation of the charge correlation function in the $4 \times 4$, $6 \times 6$, $8 \times 8$ and $10 \times 10$ clusters.

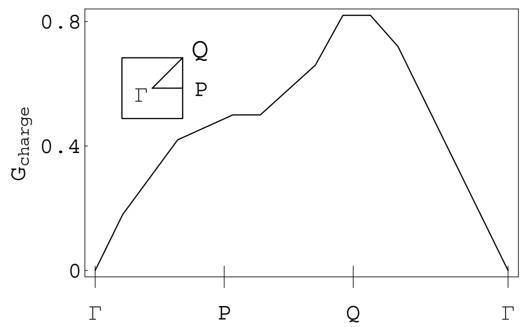



**Figure 5.** The Fourier transform of the charge correlation function in the $10 \times 10$ cluster; a delta function at the $\Gamma$ point is removed. The ticks on the $x$ axis correspond to $\Gamma$, P, Q and $\Gamma$, as usual.

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

$$\hat{T}(\boldsymbol{r})c_i^\dagger|0\rangle = \sum_{\gamma=1}^{2N-2} T(\boldsymbol{r})_{i,\gamma}c_\gamma^\dagger|0\rangle = \begin{cases} \displaystyle\sum_{\alpha=1}^{N-1} T(\boldsymbol{r})_{i,\alpha}c_\alpha^\dagger|0\rangle, & i = 1,\ldots,N-1 \\ \displaystyle\sum_{\beta=N}^{2N-2} T(\boldsymbol{r})_{i,\beta}c_\beta^\dagger|0\rangle, & i = N,\ldots,2N-2. \end{cases} \tag{A.1}$$

We have

$$\begin{aligned} \hat{T}(\boldsymbol{r})c_{1,\uparrow}^\dagger c_{1,\downarrow}|\Phi_\downarrow^{[0]}\rangle = \frac{1}{\sqrt{\mathcal{N}}} &\sum_{\alpha_1\ldots\alpha_{N-1}=1}^{N-1} \sum_{\beta_1\ldots\beta_{N-1}=N}^{2N-2} \prod_{a=1}^{N-1} T(\boldsymbol{r})_{a,\alpha_a} \prod_{b=N}^{2N-2} T(\boldsymbol{r})_{b,\beta_b} \\ &\times \sum_{k=0}^{N-2}(-)^k f_k \sum_{i_k>\cdots>i_1=2}^{N-1} \sum_{j_k>\cdots>j_1=1}^{N-1} \\ &\times \hat{S}^+_{\alpha_{i_k}}\ldots\hat{S}^+_{\alpha_{i_1}}\hat{S}^+_{\alpha_1}\hat{S}^-_{\beta_{j_k}}\ldots\hat{S}^-_{\beta_{j_1}}c^\dagger_{\alpha_1,\downarrow}\ldots c^\dagger_{\alpha_{N-1},\downarrow}c^\dagger_{\beta_1,\uparrow}\ldots c^\dagger_{\beta_{N-1},\uparrow}|0\rangle \end{aligned} \tag{A.2}$$

and hence

$$\begin{aligned} X(\boldsymbol{r}) = \frac{1}{\mathcal{N}} &\sum_{\alpha_1\ldots\alpha_{N-1}=1}^{N-1} \sum_{\beta_1\ldots\beta_{N-1}=N}^{2N-2} \prod_{a=1}^{N-1} T(\boldsymbol{r})_{a,\alpha_a} \prod_{b=N}^{2N-2} T(\boldsymbol{r})_{b,\beta_b} \sum_{k=0}^{N-2} f_k^2 \\ &\times \Bigg\{ \sum_{m_k>\cdots>m_1=2}^{N-1} \sum_{i_k>\cdots>i_1=2}^{N-1} \\ &\times \langle 0|c_{N-1,\downarrow}\ldots c_{1,\downarrow}\hat{S}^-_{m_k}\ldots\hat{S}^-_{m_1}\hat{S}^-_1\hat{S}^+_{\alpha_{i_k}}\ldots\hat{S}^+_{\alpha_{i_1}}\hat{S}^+_{\alpha_1}c^\dagger_{\alpha_1,\downarrow}\ldots c^\dagger_{\alpha_{N-1},\downarrow}|0\rangle\Bigg\} \\ &\times \Bigg\{ \sum_{n_k>\cdots>n_1=N}^{2N-2} \sum_{j_k>\cdots>j_1=1}^{N-1} \\ &\times \langle 0|c_{2N-2,\uparrow}\ldots c_{N,\uparrow}\hat{S}^+_{n_k}\ldots\hat{S}^+_{n_1}\hat{S}^-_{\beta_{j_k}}\ldots\hat{S}^-_{\beta_{j_1}}c^\dagger_{\beta_1,\uparrow}\ldots c^\dagger_{\beta_{N-1},\uparrow}|0\rangle\Bigg\}. \end{aligned} \tag{A.3}$$

Taking into account that the annihilation operators in the second and third rows 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:

$$\begin{aligned} &\sum_{i_k>\cdots>i_1=2}^{N-1} \hat{S}^+_{\alpha_{i_k}}\ldots\hat{S}^+_{\alpha_{i_1}}\hat{S}^+_{\alpha_1}c^\dagger_{\alpha_1,\downarrow}\ldots c^\dagger_{\alpha_{N-1},\downarrow}|0\rangle \\ &\qquad = \varepsilon_{\alpha_1\ldots\alpha_{N-1}} \sum_{i_k>\cdots>i_1=1,\neq\alpha_1}^{N-1} \hat{S}^+_{i_k}\ldots\hat{S}^+_{i_1}\hat{S}^+_{\alpha_1}c^\dagger_{1,\downarrow}\ldots c^\dagger_{N-1,\downarrow}|0\rangle + \cdots \end{aligned} \tag{A.4}$$

$$\begin{aligned} &\sum_{j_k>\cdots>j_1=1}^{N-1} \hat{S}^-_{\beta_{j_k}}\ldots\hat{S}^-_{\beta_{j_1}}c^\dagger_{\beta_1,\uparrow}\ldots c^\dagger_{\beta_{N-1},\uparrow}|0\rangle \\ &\qquad = \tilde{\varepsilon}_{\beta_1\ldots\beta_{N-1}} \sum_{j_k>\cdots>j_1=N}^{2N-2} \hat{S}^-_{j_k}\ldots\hat{S}^-_{j_1}c^\dagger_{N,\uparrow}\ldots c^\dagger_{2N-2,\uparrow}|0\rangle + \cdots \end{aligned} \tag{A.5}$$

where $\varepsilon$ is the totally antisymmetric tensor with $N-1$ indices, while $\tilde{\varepsilon}_{\beta_1\ldots\beta_{N-1}} \equiv \varepsilon_{\beta_1-N+1\cdots\beta_{N-1}-N+1}$ and the dots mean that we are neglecting other terms whose contribution to the scalar product is zero. On the right-hand side of equation (A.4) 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 equation (A.4), the second row of equation (A.3) yields

$$\varepsilon_{\alpha_1\ldots\alpha_{N-1}} \sum_{m_k>\cdots>m_1=2}^{N-1} \sum_{i_k>\cdots>i_1=1,\neq\alpha_1}^{N-1} \langle 0|c_{N-1,\downarrow}\ldots c_{1,\downarrow}\hat{S}^-_{m_k}\ldots\hat{S}^-_{m_1}\hat{S}^-_1\hat{S}^+_{i_k}\ldots\hat{S}^+_{i_1}\hat{S}^+_{\alpha_1}c^\dagger_{1,\downarrow}\ldots c^\dagger_{N-1,\downarrow}|0\rangle$$
$$= \varepsilon_{\alpha_1\ldots\alpha_{N-1}}\left[\delta_{1\alpha_1}\binom{N-2}{k} + (1-\delta_{1\alpha_1})\binom{N-3}{k-1}\right] \tag{A.6}$$

while using equation (A.5), the third row of equation (A.3) yields

$$\tilde{\varepsilon}_{\beta_1\ldots\beta_{N-1}} \sum_{n_k>\cdots>n_1=N}^{2N-2} \sum_{j_k>\cdots>j_1=N}^{2N-2} \langle 0|c_{2N-2,\uparrow}\ldots c_{N,\uparrow}\hat{S}^+_{n_k}\ldots\hat{S}^+_{n_1}\hat{S}^-_{j_k}\ldots\hat{S}^-_{j_1}c^\dagger_{N,\uparrow}\ldots c^\dagger_{2N-2,\uparrow}|0\rangle$$
$$= \tilde{\varepsilon}_{\beta_1\ldots\beta_{N-1}}\binom{N-1}{k}. \tag{A.7}$$

These two last results allow us to rewrite $X(\boldsymbol{r})$ as

$$X(\boldsymbol{r}) = \frac{A}{|\mathcal{S}_{hf}|^2} + B\mathcal{C}_{1,1}(\boldsymbol{r})T(\boldsymbol{r})_{1,1} \tag{A.8}$$

where, using the convention $\binom{r}{-|s|} = 0$ for a binomial coefficient with negative down entry,

$$\boxed{A = \frac{|\mathcal{S}_{hf}|^2}{\mathcal{N}}\sum_{k=0}^{N-2} f_k^2\binom{N-1}{k}\binom{N-3}{k-1}} \tag{A.9}$$

$$\boxed{B = \frac{1}{\mathcal{N}}\sum_{k=0}^{N-2} f_k^2\binom{N-1}{k}\left[\binom{N-2}{k}\binom{N-3}{k-1}\right]} \tag{A.10}$$

and $\mathcal{C}_{1,1}(\boldsymbol{r})$ is the (1, 1) algebraic complement of the matrix $T(\boldsymbol{r})$ whose determinant is equal to unity for even $x+y$. The (1, 1) algebraic complement can be expressed in terms of the (1, 1) element of the matrix $T(\boldsymbol{r})$: $\mathcal{C}_{1,1}(\boldsymbol{r}) = T^\dagger(\boldsymbol{r})_{1,1}\mathrm{Det}[T(\boldsymbol{r})] = T(\boldsymbol{r})_{1,1}$ (since $T(\boldsymbol{r})_{i,j} \in \Re$). Next one has to recognize that $T(\boldsymbol{r})_{1,1}$ is, by definition, equal to $t_1(\boldsymbol{r})$ (see equation (46)) whose analytic expression is given in equation (53). Therefore, any time $x+y$ is even we have

$$\boxed{X(\boldsymbol{r}) = \frac{1}{|\mathcal{S}_{hf}|^2}[A + B\times\mathcal{T}_{hf}(\boldsymbol{r})^2].} \tag{A.11}$$

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

$$\hat{T}(\boldsymbol{r})c^\dagger_i|0\rangle = \sum_{\gamma=1}^{2N-2} T(\boldsymbol{r})_{i,\gamma}c^\dagger_\gamma|0\rangle = \begin{cases} \displaystyle\sum_{\alpha=N}^{2N-2} T(\boldsymbol{r})_{i,\alpha}c^\dagger_\alpha|0\rangle, & i = 1,\ldots,N-1 \\ \displaystyle\sum_{\beta=1}^{N-1} T(\boldsymbol{r})_{i,\beta}c^\dagger_\beta|0\rangle, & i = N,\ldots,2N-2 \end{cases} \tag{A.12}$$

and hence

$$\hat{T}(\boldsymbol{r})c^\dagger_{1,\uparrow}c_{1,\downarrow}|\Phi^{[0]}_\downarrow\rangle = \frac{1}{\sqrt{\mathcal{N}}}\sum_{\alpha_1\ldots\alpha_{N-1}=N}^{2N-2}\sum_{\beta_1\ldots\beta_{N-1}=1}^{N-1}\prod_{a=1}^{N-1}T(\boldsymbol{r})_{a,\alpha_a}\prod_{b=N}^{2N-2}T(\boldsymbol{r})_{b,\beta_b}$$
$$\times\sum_{k=0}^{N-2}(-)^k f_k \sum_{i_k>\cdots>i_1=2}^{N-1}\sum_{j_k>\cdots>j_1=1}^{N-1}$$
$$\times\hat{S}^+_{\alpha_{i_k}}\ldots\hat{S}^+_{\alpha_{i_1}}\hat{S}^+_{\alpha_1}\hat{S}^-_{\beta_{j_k}}\ldots\hat{S}^-_{\beta_{j_1}}c^\dagger_{\alpha_1,\downarrow}\ldots c^\dagger_{\alpha_{N-1},\downarrow}c^\dagger_{\beta_1,\uparrow}\ldots c^\dagger_{\beta_{N-1},\uparrow}|0\rangle. \tag{A.13}$$

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 $c^{\dagger}_{1,\uparrow}c_{1,\downarrow}|\Phi^{[0]}_{\downarrow}\rangle$ originates from the $(N-k-2)$th term of the corresponding expansion (see equation (50)). Hence

$$X(\boldsymbol{r}) = -\frac{1}{\mathcal{N}} \sum_{\alpha_1\ldots\alpha_{N-1}=N}^{2N-2} \sum_{\beta_1\ldots\beta_{N-1}=1}^{N-1} \prod_{a=1}^{N-1} T(\boldsymbol{r})_{a,\alpha_a} \prod_{b=N}^{2N-2} T(\boldsymbol{r})_{b,\beta_b} \sum_{k=0}^{N-2} f_k f_{N-k-2}$$
$$\times \left\{ \sum_{m_{N-k-2}>\cdots>m_1=2}^{N-1} \sum_{j_k>\cdots>j_1=1}^{N-1} \right.$$
$$\left. \times \langle 0|c_{N-1,\downarrow}\ldots c_{1,\downarrow}\hat{S}^{-}_{m_{N-k-2}}\ldots\hat{S}^{-}_{m_1}\hat{S}^{-}_{1}\hat{S}^{-}_{\beta_{j_k}}\ldots\hat{S}^{-}_{\beta_{j_1}}c^{\dagger}_{\beta_1,\uparrow}\ldots c^{\dagger}_{\beta_{N-1},\uparrow}|0\rangle \right\}$$
$$\times \left\{ \sum_{n_{N-k-2}>\cdots>n_1=N}^{2N-2} \sum_{i_k>\cdots>i_1=2}^{N-1} \right.$$
$$\left. \times \langle 0|c_{2N-2,\uparrow}\ldots c_{N,\uparrow}\hat{S}^{+}_{n_{N-k-2}}\ldots\hat{S}^{+}_{n_1}\hat{S}^{+}_{\alpha_{i_k}}\ldots\hat{S}^{+}_{\alpha_{i_1}}\hat{S}^{+}_{\alpha_1}c^{\dagger}_{\alpha_1,\downarrow}\ldots c^{\dagger}_{\alpha_{N-1},\downarrow}|0\rangle \right\}. \tag{A.14}$$

Analogously to the case $x+y$ even, the particular structure of $|\Phi^{[0]}_{AF}\rangle$ allows the following simplification:

$$\sum_{j_k>\cdots>j_1=1}^{N-1} \hat{S}^{-}_{\beta_{j_k}}\ldots\hat{S}^{-}_{\beta_{j_1}}c^{\dagger}_{\beta_1,\uparrow}\ldots c^{\dagger}_{\beta_{N-1},\uparrow}|0\rangle$$
$$= \varepsilon_{\beta_1\ldots\beta_{N-1}} \sum_{j_k>\cdots>j_1=1}^{N-1} \hat{S}^{-}_{j_k}\ldots\hat{S}^{-}_{j_1}c^{\dagger}_{1,\uparrow}\ldots c^{\dagger}_{N-1,\uparrow}|0\rangle + \cdots \tag{A.15}$$

$$\sum_{i_k>\cdots>i_1=2}^{N-1} \hat{S}^{+}_{\alpha_{i_k}}\ldots\hat{S}^{+}_{\alpha_{i_1}}\hat{S}^{+}_{\alpha_1}c^{\dagger}_{\alpha_1,\downarrow}\ldots c^{\dagger}_{\alpha_{N-1},\downarrow}|0\rangle$$
$$= \tilde{\varepsilon}_{\alpha_1\ldots\alpha_{N-1}} \sum_{i_k>\cdots>i_1=N,\neq\alpha_1}^{2N-2} \hat{S}^{+}_{i_k}\ldots\hat{S}^{+}_{i_1}\hat{S}^{+}_{\alpha_1}c^{\dagger}_{N,\downarrow}\ldots c^{\dagger}_{2N-2,\downarrow}|0\rangle\ldots \tag{A.16}$$

where $\tilde{\varepsilon}_{\alpha_1\ldots\alpha_{N-1}} = \varepsilon_{\alpha_1-N+1\ldots\alpha_{N-1}-N+1}$ and the sum on the right-hand side of equation (A.16) means that the indices $i_k > \cdots > i_1$ run in the interval $\{N,\ldots,2N-2\}$ in such a way that none of them is equal to $\alpha_1$. All the neglected terms contribute nothing to the scalar product.

Using equation (A.15) the second row of (A.14) yields

$$\varepsilon_{\beta_1\ldots\beta_{N-1}} \sum_{m_{N-k-2}>\cdots>m_1=2}^{N-1} \sum_{j_k>\cdots>j_1=1}^{N-1} \langle 0|c_{N-1,\downarrow}\ldots c_{1,\downarrow}\hat{S}^{-}_{m_{N-k-2}}\ldots\hat{S}^{-}_{m_1}\hat{S}^{-}_{1}\hat{S}^{-}_{j_k}\ldots\hat{S}^{-}_{j_1}c^{\dagger}_{1,\uparrow}\ldots c^{\dagger}_{N-1,\uparrow}|0\rangle$$
$$= \varepsilon_{\beta_1\ldots\beta_{N-1}} \binom{N-2}{k} \tag{A.17}$$

while using equation (A.16) the third row of (A.14) yields

$$\tilde{\varepsilon}_{\alpha_1\ldots\alpha_{N-1}} \sum_{n_{N-k-2}>\cdots>n_1=N}^{2N-2} \sum_{i_k>\cdots>i_1=N,\neq\alpha_1}^{2N-2}$$
$$\times \langle 0|c_{2N-2,\uparrow}\ldots c_{N,\uparrow}\hat{S}^{+}_{n_{N-k-2}}\ldots\hat{S}^{+}_{n_1}\hat{S}^{+}_{i_k}\ldots\hat{S}^{+}_{i_1}\hat{S}^{+}_{\alpha_1}c^{\dagger}_{N,\downarrow}\ldots c^{\dagger}_{2N-2,\downarrow}|0\rangle$$
$$= \tilde{\varepsilon}_{\alpha_1\ldots\alpha_{N-1}} \binom{N-2}{k}. \tag{A.18}$$

Substituting these results in the expression for $X(\boldsymbol{r})$ we obtain

$$\boxed{X(\boldsymbol{r}) = -\frac{C}{|\mathcal{S}_{hf}|^2} = -\frac{1}{|\mathcal{S}_{hf}|^2}[A + B \times (4N-4)]} \tag{A.19}$$

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

$$\boxed{C = \frac{|\mathcal{S}_{hf}|^2}{\mathcal{N}} \sum_{k=0}^{N-2} f_k f_{N-k-2} \binom{N-2}{k}^2.} \tag{A.20}$$

In the last equality of equation (A.19) we have used $C = A + B \times (4N-4)$, which is a direct consequence of the sum rule for the spin correlation function (see equation (58)).

## Appendix B. Evaluation of $Y$

Here we show that $Y(\boldsymbol{r}) \equiv \langle \Phi_{\uparrow}^{[0]} | \hat{T}(\boldsymbol{r}) | \Phi_{\uparrow}^{[0]} \rangle$ has the form shown in equation (80) and we derive the explicit values for the two constants $D$ and $E$. As for $X(\boldsymbol{r})$ we shall first consider the case $x+y$ even and thereafter the case $x+y$ odd. Making use of equation (A.1), we obtain

$$\begin{aligned}
\hat{T}(\boldsymbol{r})|\Phi_{\uparrow}^{[0]}\rangle = \frac{1}{\sqrt{\mathcal{N}}} & \sum_{\alpha_1\ldots\alpha_{N-1}=1}^{N-1} \sum_{\beta_1\ldots\beta_{N-1}=N}^{2N-2} \prod_{a=1}^{N-1} T(\boldsymbol{r})_{a,\alpha_a} \prod_{b=N}^{2N-2} T(\boldsymbol{r})_{b,\beta_b} \\
& \times \sum_{k=0}^{N-2} (-1)^k f_k \sum_{i_k>\cdots>i_1=2}^{N-1} \sum_{j_k>\cdots>j_1=1}^{N-1} \\
& \times \hat{S}^-_{\alpha_{i_k}} \ldots \hat{S}^-_{\alpha_{i_1}} \hat{S}^+_{\beta_{j_k}} \ldots \hat{S}^+_{\beta_{j_1}} c^\dagger_{\alpha_1,\uparrow} \ldots c^\dagger_{\alpha_{N-1},\uparrow} c^\dagger_{\beta_N,\downarrow} \ldots c^\dagger_{\beta_{2N-2},\downarrow} |0\rangle.
\end{aligned} \tag{B.1}$$

The $k$th term in the sum of equation (B.1) gives non-vanishing scalar product only with the $k$th term in equation (49) and hence

$$\begin{aligned}
Y(\boldsymbol{r}) = \frac{1}{\mathcal{N}} & \sum_{\alpha_1\ldots\alpha_{N-1}=1}^{N-1} \sum_{\beta_1\ldots\beta_{N-1}=N}^{2N-2} \prod_{a=1}^{N-1} T(\boldsymbol{r})_{a,\alpha_a} \prod_{b=N}^{2N-2} T(\boldsymbol{r})_{b,\beta_b} \sum_{k=0}^{N-2} f_k^2 \Bigg\{ \sum_{m_k>\cdots>m_1=2}^{N-1} \sum_{i_k>\cdots>i_1=2}^{N-1} \\
& \times \langle 0| c_{N-1,\uparrow} \ldots c_{1,\uparrow} \hat{S}^+_{m_k} \ldots \hat{S}^+_{m_1} \hat{S}^-_{\alpha_{i_k}} \ldots \hat{S}^-_{\alpha_{i_1}} c^\dagger_{\alpha_1,\uparrow} \ldots c^\dagger_{\alpha_{N-1},\uparrow} |0\rangle \Bigg\} \\
& \times \Bigg\{ \sum_{n_k>\cdots>n_1=N}^{2N-2} \sum_{j_k>\cdots>j_1=1}^{N-1} \\
& \times \langle 0| c_{2N-2,\downarrow} \ldots c_{N,\downarrow} \hat{S}^-_{n_k} \ldots \hat{S}^-_{n_1} \hat{S}^+_{\beta_{j_k}} \ldots \hat{S}^+_{\beta_{j_1}} c^\dagger_{\beta_1,\downarrow} \ldots c^\dagger_{\beta_{N-1},\downarrow} |0\rangle \Bigg\}.
\end{aligned} \tag{B.2}$$

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

$$\begin{aligned}
& \sum_{i_k>\cdots>i_1=2}^{N-1} \hat{S}^-_{\alpha_{i_k}} \ldots \hat{S}^-_{\alpha_{i_1}} c^\dagger_{\alpha_1,\uparrow} \ldots c^\dagger_{\alpha_{N-1},\uparrow} |0\rangle \\
& \qquad = \varepsilon_{\alpha_1\ldots\alpha_{N-1}} \sum_{i_k>\cdots>i_1=1,\neq\alpha_1}^{N-1} \hat{S}^-_{i_1} \ldots \hat{S}^-_{i_k} c^\dagger_{1,\uparrow} \ldots c^\dagger_{N-1,\uparrow} |0\rangle + \cdots
\end{aligned} \tag{B.3}$$

where the neglected terms do not contribute to the scalar product. In the second row of equation (B.2), $c_{1,\uparrow}$ commutes with all the raising spin operators whatever are the values of the $k$ indices $m_k > \cdots > m_1$ in the range specified by the sum. This implies that $i_1$ cannot be unity. On the other hand $c^\dagger_{\alpha_1}$ commutes with all the lowering spin operators and hence no one of the indices $m_k > \cdots > m_1$ can be $\alpha_1$ otherwise the corresponding term vanishes. Hence the term in the second row gives

$$\sum_{m_k>\cdots>m_1=2,\neq\alpha_1}^{N-1} \sum_{i_k>\cdots>i_1=2,\neq\alpha_1}^{N-1} \varepsilon_{\alpha_1\ldots\alpha_{N-1}} \langle 0|c_{N-1,\uparrow}\ldots c_{1,\uparrow}\hat{S}^+_{m_k}\ldots\hat{S}^+_{m_1}\hat{S}^-_{i_1}\ldots\hat{S}^-_{i_k}c^\dagger_{1,\uparrow}\ldots c^\dagger_{N-1,\uparrow}|0\rangle$$
$$= \left[\sum_{i_k>\cdots>i_1=2,\neq\alpha_1}^{N-1}\right]\varepsilon_{\alpha_1\ldots\alpha_{N-1}}. \tag{B.4}$$

If $k = N-2$ the sum is zero except for $\alpha_1 = 1$ since the indices $i_k > \cdots > i_1$ do not have space to run. Hence

$$\sum_{i_k>\cdots>i_1=2,\neq\alpha_1}^{N-1} = \delta_{k,N-2}\delta_{1,\alpha_1} + (1-\delta_{k,N-2})\left[\binom{N-3}{k} + \delta_{1,\alpha_1}\left(\binom{N-2}{k} - \binom{N-3}{k}\right)\right]$$
$$= (1-\delta_{k,N-2})\binom{N-3}{k}$$
$$+\delta_{1,\alpha_1}\left[\delta_{k,N-2} + (1-\delta_{k,N-2})\left(\binom{N-2}{k} - \binom{N-3}{k}\right)\right] \tag{B.5}$$

while the third row of equation (B.2) yields

$$\tilde{\varepsilon}_{\beta_1\ldots\beta_{N-1}} \sum_{n_k>\cdots>n_1=N}^{2N-2} \sum_{j_k>\cdots>j_1=N}^{2N-2} \langle 0|c_{2N-2,\downarrow}\ldots c_{N,\downarrow}\hat{S}^-_{n_k}\ldots\hat{S}^-_{n_1}\hat{S}^+_{j_k}\ldots\hat{S}^+_{j_1}c^\dagger_{N,\downarrow}\ldots c^\dagger_{2N-2,\downarrow}|0\rangle$$
$$= \tilde{\varepsilon}_{\beta_1\ldots\beta_{N-1}}\binom{N-1}{k} \tag{B.6}$$

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

$$\boxed{Y(\boldsymbol{r}) = \frac{1}{4} + \frac{D}{|\mathcal{S}_{hf}|^2} + E\mathcal{C}_{1,1}(\boldsymbol{r})T(\boldsymbol{r})_{1,1} = \frac{1}{4} + \frac{1}{|\mathcal{S}_{hf}|^2}[D + E\times\mathcal{T}_{hf}(\boldsymbol{r})^2],} \tag{B.7}$$

where $D$ and $E$ are two $N$-dependent constants given by

$$\boxed{D = \frac{|\mathcal{S}_{hf}|^2}{\mathcal{N}}\left[\sum_{k=0}^{N-3} f_k^2\binom{N-1}{k}\binom{N-3}{k} - \frac{\mathcal{N}}{4}\right]} \tag{B.8}$$

$$\boxed{E = \frac{1}{\mathcal{N}}\left\{(N-1)f_{N-2}^2 + \sum_{k=1}^{N-3} f_k^2\binom{N-1}{k}\left[\binom{N-2}{k} - \binom{N-3}{k}\right]\right\}.} \tag{B.9}$$

For odd $x+y$ we make use of equation (A.12). Then, the action of $\hat{T}(\boldsymbol{r})$ over $|\Phi^{[0]}_\uparrow\rangle$ gives

$$\hat{T}(\boldsymbol{r})|\Phi^{[0]}_\uparrow\rangle = \frac{1}{\sqrt{\mathcal{N}}}\sum_{\alpha_1\ldots\alpha_{N-1}=N}^{2N-2}\sum_{\beta_1\ldots\beta_{N-1}=1}^{N-1}\prod_{a=1}^{N-1}T(\boldsymbol{r})_{a,\alpha_a}\prod_{b=N}^{2N-2}T(\boldsymbol{r})_{b,\beta_b}$$
$$\times\sum_{k=0}^{N-2}(-)^k f_k\sum_{i_k>\cdots>i_1=2}^{N-1}\sum_{j_k>\cdots>j_1=1}^{N-1}$$
$$\times\hat{S}^-_{\alpha_{i_k}}\ldots\hat{S}^-_{\alpha_{i_1}}\hat{S}^+_{\beta_{j_k}}\ldots\hat{S}^+_{\beta_{j_1}}c^\dagger_{\alpha_1,\uparrow}\ldots c^\dagger_{\alpha_{N-1},\uparrow}c^\dagger_{\beta_1,\downarrow}\ldots c^\dagger_{\beta_{N-1},\downarrow}|0\rangle. \tag{B.10}$$

In the scalar product with the $|\Phi_{\uparrow}^{[0]}\rangle$ 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 equation (B.10); 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 $|\Phi_{\uparrow}^{[0]}\rangle$, equation (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

$$\begin{aligned}
Y(\boldsymbol{r}) = \frac{1}{\mathcal{N}} &\sum_{\alpha_1\ldots\alpha_{N-1}=N}^{2N-2} \sum_{\beta_1\ldots\beta_{N-1}=1}^{N-1} \prod_{a=1}^{N-1} T(\boldsymbol{r})_{a,\alpha_a} \prod_{b=N}^{2N-2} T(\boldsymbol{r})_{b,\beta_b} \sum_{k=1}^{N-2} f_k f_{N-k-1} \\
&\times \Bigg\{ \sum_{m_{N-k-1}>\cdots>m_1=2}^{N-1} \sum_{j_k>\cdots>j_1=1}^{N-1} \\
&\times \langle 0|c_{N-1,\uparrow}\ldots c_{1,\uparrow}\hat{S}^+_{m_{N-k-1}}\ldots\hat{S}^+_{m_1}\hat{S}^+_{\beta_{j_k}}\ldots\hat{S}^+_{\beta_{j_1}}c^\dagger_{\beta_1\downarrow}\ldots c^\dagger_{\beta_{N-1}\downarrow}|0\rangle\Bigg\} \\
&\times \Bigg\{ \sum_{n_{N-k-1}>\cdots>n_1=N}^{2N-2} \sum_{i_k>\cdots>i_1=2}^{N-1} \\
&\times \langle 0|c_{2N-2,\downarrow}\ldots c_{N,\downarrow}\hat{S}^-_{n_{N-k-1}}\ldots\hat{S}^-_{n_1}\hat{S}^-_{\alpha_{i_k}}\ldots\hat{S}^-_{\alpha_{i_1}}c^\dagger_{\alpha_1,\uparrow}\ldots c^\dagger_{\alpha_{N-1},\uparrow}|0\rangle\Bigg\}.
\end{aligned} \qquad \text{(B.11)}$$

Let us consider the term in the second row. For a given choice of $\beta_1\ldots\beta_{N-1}$ one finds

$$\begin{aligned}
&\sum_{j_k>\cdots>j_1=1}^{N-1} \hat{S}^+_{\beta_{j_k}}\ldots\hat{S}^+_{\beta_{j_1}}c^\dagger_{\beta_1\downarrow}\ldots c^\dagger_{\beta_{N-1}\downarrow}|0\rangle \\
&\qquad = \varepsilon_{\beta_1\ldots\beta_{N-1}} \sum_{j_k>\cdots>j_1=1}^{N-1} \hat{S}^+_{j_k}\ldots\hat{S}^+_{j_1}c^\dagger_{1,\downarrow}\ldots c^\dagger_{N-1,\downarrow}|0\rangle + \cdots,
\end{aligned} \qquad \text{(B.12)}$$

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 originating from the sum over $m_{N-k-1} > \cdots > m_1$, $j_1$ is constrained to be unity for all non-vanishing contributions. Still for $j_k > \cdots > j_2$ fixed there is only one choice for $m_{N-k-1} > \cdots > m_1$ to have non-vanishing result. In particular, the possible results for a given choice of $j_k > \cdots > j_2$ and $m_{N-k-1} > \cdots > m_1$ are zero or unity. Hence the term in the first square bracket yields

$$\begin{aligned}
&\varepsilon_{\beta_1\ldots\beta_{N-1}} \sum_{m_{N-k-1}>\cdots>m_1=2}^{N-1} \sum_{j_k>\cdots>j_2=2}^{N-1} \langle 0|c_{N-1,\uparrow}\ldots c_{1,\uparrow}\hat{S}^+_{m_{N-k-1}}\ldots\hat{S}^+_{m_1}\hat{S}^+_{j_k}\ldots\hat{S}^+_{j_1}c^\dagger_{1,\downarrow}\ldots c^\dagger_{N-1,\downarrow}|0\rangle \\
&\qquad = \varepsilon_{q_1\ldots q_{N-1}} \binom{N-2}{k-1}.
\end{aligned} \qquad \text{(B.13)}$$

A similar trick can be used for the term in the third row of equation (B.11). We obtain

$$\begin{aligned}
&\sum_{i_k>\cdots>i_1=2}^{N-1} \hat{S}^-_{\alpha_{i_k}}\ldots\hat{S}^-_{\alpha_{i_1}}c^\dagger_{\alpha_1,\uparrow}\ldots c^\dagger_{\alpha_{N-1},\uparrow}|0\rangle \\
&\qquad = \tilde{\varepsilon}_{\alpha_1\ldots\alpha_{N-1}} \sum_{i_k>\cdots>i_1=N,\neq\alpha_1}^{2N-2} \hat{S}^-_{i_k}\ldots\hat{S}^-_{i_1}c^\dagger_{N,\uparrow}\ldots c^\dagger_{2N-2,\uparrow}|0\rangle + \cdots.
\end{aligned} \qquad \text{(B.14)}$$

Since the $c^\dagger_{\alpha_1,\uparrow}$ creation operator commutes with all the lowering spin operators originating from the sum over $i_k > \cdots > i_1$, one of the indices $n_{N-k-1} > \cdots > n_1$ is constrained to be

$\alpha_1$ and the third row of equation (B.11) can be rewritten as

$$\tilde{\varepsilon}_{\alpha_1\ldots\alpha_{N-1}} \sum_{n_{N-k-1}>\cdots>n_2=N,\neq\alpha_1}^{2N-2} \sum_{i_k>\cdots>i_1=N,\neq\alpha_1}^{2N-2} \times\langle 0|c_{2N-2,\downarrow}\ldots c_{N,\downarrow}\hat{S}^-_{n_{N-k-1}}\ldots\hat{S}^-_{n_1}\hat{S}^-_{i_k}\ldots\hat{S}^-_{i_1}c^\dagger_{N,\uparrow}\ldots c^\dagger_{2N-2,\uparrow}|0\rangle = \begin{pmatrix} N-2 \\ k \end{pmatrix}\tilde{\varepsilon}_{\alpha_1\ldots\alpha_{N-1}}. \tag{B.15}$$

Substituting these results in equation (B.11) one obtains

$$\boxed{Y(\boldsymbol{r}) = \frac{F_N}{|\mathcal{S}_{hf}|^2} = \frac{1}{4} - \frac{1}{|\mathcal{S}_{hf}|^2}[D + E\times(4N-4)]} \tag{B.16}$$

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

$$\boxed{F_N = \frac{|\mathcal{S}_{hf}|^2}{\mathcal{N}}\sum_{k=1}^{N-2} f_k f_{N-k-1}\begin{pmatrix} N-2 \\ k-1 \end{pmatrix}\begin{pmatrix} N-2 \\ k \end{pmatrix}.} \tag{B.17}$$

In the last equality of equation (B.16) we have used $F_N = |\mathcal{S}_{hf}|^2/4 - D - E\times(4N-4)$, which is a direct consequence of the sum rule for the charge correlation function (see equation (81)).

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