Formation probabilities and statistics of observables as defect problems in the free fermions and the quantum spin chains

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We show that the computation of formation probabilities (FP) in the configuration basis and the full counting statistics (FCS) of observables in the quadratic fermionic Hamiltonians are equivalent to the calculation of emptiness formation probability (EFP) in the Hamiltonian with a defect. In particular, we first show that the FP of finding a particular configuration in the ground state is equivalent to the EFP of the ground state of the quadratic Hamiltonian with a defect. Then, we show that the probability of finding a particular value for any quadratic observable is equivalent to a FP problem and ultimately leads to the calculation of EFP in the ground state of a Hamiltonian with a defect. We provide new exact determinant formulas for the FP in the generic quadratic fermionic Hamiltonians. As applications of our formalism we study the statistics of the number of particles and kinks. Our conclusions can be extended also to the quantum spin chains that can be mapped to the free fermions via Jordan-Wigner (J-W) transformation. In particular, we provide an exact solution to the problem of the transverse field XY chain with a staggered line defect. We also study the distribution of magnetization and kinks in the transverse field XY chain and show how the dual nature of these quantities manifest itself in the distributions.
I. INTRODUCTION

Consider a quantum many body state written in a configuration basis, then the formation probability of a particular configuration in a subsystem is the probability of finding the configuration if we do the measurement in that particular basis. For example, if we take the ground state of a spinless fermionic system and ask the same question for the subsystem $D$ then there are $2^{|D|}$ possibilities for the configurations, where $|D|$ is the size of the subsystem. Every configuration appears with a particular probability which we call formation probability. The simplest example of the FP is the emptiness formation probability which is about the FP of the configuration without any fermion in the subsystem and has a long history. It was studied in the context of the XXZ spin chain in $9-12$. FP has been also studied from the conformal field theory (CFT) point of view in $13-16$. The problem is related to the solution of the free energy of a quantum field theory with a slit which in the context of the CFT studied in $17$ and references therein. A relation to the Casimir energy problem is also established in $14,15$. The FP can be also used to find the Shannon entropy with plethora of applications in the studies of quantum phase transitions, see $18-28$.

One can also look to the problem of the FP from a different point of view. Consider a configuration basis which is associated with the local on-site observable $\hat{o}_i$ at site $i$ with eigenvalues(eigenvectors) $o^j_i(|a^j_i\rangle)$, $j = 1, 2, ..., d$, where $d$ is the dimension of the local on-site Hilbert space. Then one can define an on-site projection operator as $\pi^j_i = |o^j_i\rangle\langle o^j_i|$. Multiplication of these operators in a subsystem leads to a projection operator $\Pi^j_0 = \prod_i \pi^j_i$, where the set $\{j\}$ fix the configuration by picking a particular $\pi^j_i$ at every site. Finally the average over, for example, the ground state $|g\rangle$ of the Hamiltonian $H$ gives the FP for the desired configuration, i.e. $P(\{j\}) = \langle g|\Pi^j_0|g\rangle$. Now consider one primitive configuration with all the sites being in the eigenstate corresponding to, for example, $o^i$ i.e. $|\{1\}\rangle$. In the case of fermions this primitive configuration can be the configuration without fermions. Then one can always find a unitary similarity transformation matrix $T^{(j)}$ which $P(\{j\}) = \langle g' |\Pi_0^{(1)}|g'\rangle$, where $|g'\rangle = T^{(j)}|g\rangle$. The state $|g'\rangle$ can be considered as the ground state of the Hamiltonian $H' = T^{(j)}H(T^{(j)})^{-1}$ which is basically the same Hamiltonian as $H$ but with a line defect. This simple argument shows that formally one can look to the problem of generic FP as the problem of the probability of a primitive configuration in the deformed Hamiltonian. Many body systems with line defects have been studied for decades, for some earlier studies see for example $13-16$. For studies related to boundary CFT and integrable quantum field theories see $35-43$ and $44$.

In a different approach to the above one could also define the generating function $M(\{\lambda_i\}) = \langle e^{\sum_i \lambda_i \hat{o}_i} \rangle$, where the coefficients of the exponentials are the FP’s. This is a non-trivial example of a more widely known concept called full counting statistics which deals with the fluctuations of an observable defined in a subsystem. In most of the FCS problems one is interested in the moments of an observable $\hat{O}$ defined for the entire subsystem, i.e. $\langle \hat{O}^n \rangle$. Being a very natural concept FCS has been studied for a long time in different communities. It has been studied in the context of charge fluctuations $45,46$, Bose gases $47-51$, particle number fluctuations $52-56$, quantum spin chains $57-64$ and out of equilibrium quantum systems $51,65,66$.

It is not difficult to see that the FCS of an observable defined in a subsystem can be formulated as a formation probability problem by just considering the basis that diagonalizes the observable $\hat{O}$. In this basis one can consider every eigenstate of the observable as a configuration and then the probability to find a particular value for the observable is just the FP for that configuration. This connection seems too formal to be useful, however, in this article we show that this point of view is extremely useful when one deals with quadratic observables in the study of FCS in the quadratic fermion Hamiltonians and the corresponding spin chains. The main advantage with respect to the more standard generating function point of view is that here one does not need to do the inverse Laplace transformation which is normally impossible to do analytically. Even numerical calculation of such kind of inverse transformation is usually extremely difficult because of the presence of a square root of a determinant in the final result of the generating function. Apart from its conceptual appeal our approach provides an explicit formula for the probabilities which is its main advantage with respect to the generating function method.

The paper is organized as follows: In the next section we first introduce the concept of FP and EFP in the quadratic Hamiltonians. Then we provide new determinant formulas for the FP and show explicitly how the FP is an EFP for the Hamiltonian with a defect, a line defect in the case of one dimensional systems. In section III we study the statistics of quadratic observables and show that this problem is related to the FP and ultimately EFP of a Hamiltonian with defect. A couple of examples including the number of particles and kinks will be discussed briefly. In section IV we study the transverse field XY chain with a staggered line defect. We find the exact correlation matrix of this Hamiltonian and argue that our result is valid for a generic translational invariant quadratic fermion Hamiltonian with a staggered line defect. In section V we use the general equations introduced in section III to calculate the probability distribution of the particle numbers and kinks in the transverse field XY chain. Finally in section VI we summarize our findings and comment on the future directions.
II. FORMATION PROBABILITY AS EMPTINESS FORMATION PROBABILITY

Consider the following free fermion Hamiltonian with real generic couplings:

\[ \mathcal{H}_{\text{free}}(A, B) = c^\dagger A c + \frac{1}{2} c^\dagger B c + \frac{1}{2} c B^T c - \frac{1}{2} \text{Tr} A, \]  

(1)

where \( A \) and \( B \) are symmetric and anti-symmetric matrices respectively and \( c = (c_1, c_2, \ldots, c_D) \) with similar definition for \( c^\dagger \). We define the correlation matrix of the ground state of the above Hamiltonian as:

\[ i G_{jk} = \langle \bar{\gamma}_j \gamma_k \rangle, \]  

(2)

where we defined the Majorana operators \( \gamma_k = c_k + c_k^\dagger \) and \( \bar{\gamma}_j = i(c_j^\dagger - c_j) \) and \( \langle \rangle \) is normally the expectation value in the ground state. Note that here we have \( \delta_{jk} = \langle \bar{\gamma}_j \gamma_k \rangle = -\langle \bar{\gamma}_j^\dagger \gamma_k^\dagger \rangle \). Using the Wick’s theorem which is valid for the eigenstates of the above Hamiltonian one can write all the other correlation functions with respect to these three basic correlation functions. Other interesting quantities such as entanglement entropy and FP’s can be also written as a function of the correlation matrix. Intuitively FP is defined as the probability of finding a particular configuration \( C \) in a subsystem of the full system. It was shown in\(^1\) that the result can be written with respect to the correlation matrix as follows:

\[ P(C) = \det \frac{I - G}{2} \text{Min}[F], \]  

(3)

where Min\( F \) is a particular principal minor of the matrix \( F = \frac{1}{2} I + G \) derived after removing the rows and columns of the sites without any fermion in the configuration \( C \). When there is no fermion in the configuration \( C \) then the corresponding probability is called emptiness formation probability and we have

\[ P(\{\emptyset\}) = \det \frac{I - G}{2}, \]  

(4)

whereas when all the sites are occupied with fermions we have

\[ P(\{\{\}\}) = \det \frac{I + G}{2}. \]  

(5)

The above two formulas are very useful equations to do analytical calculations when there is a translational invariance. However, because of the presence of the minor in the equation (3) analytical calculations do not seem to be feasible in more generic cases. One way to overcome this problem can be mapping the problem of FP to the problem of EFP and see the outcome. This procedure can be done as follows: Consider the formation probability, i.e. \( P(C) \), of the ground state of the Hamiltonian \( \mathcal{H}_{\text{free}}(A, B) \). This probability is equal to the EFP of the ground state of the Hamiltonian \( \mathcal{H}_{\text{free}}(A', B') \) with a defect. In section IV we show for an explicit example how this procedure can be followed. Finally we have:

\[ P(C) = \det \frac{I - G'}{2}, \]  

(6)

where \( G' \) is the correlation matrix of the Hamiltonian with defects. Following\(^67\) one can, in principle, find this correlation matrix numerically for any values of the coupling constants. However, analytical calculations are commonly feasible when we have translational invariance or some extra structure. For example, the Hamiltonian of a translational invariant (periodic) free fermions with time-reversal symmetry can be written as

\[ H = \sum_{r=-R}^{R} \sum_{j \in \Lambda} a_r c_j^\dagger c_{j+r} + \frac{b_r}{2} (c_j^\dagger c_{j+r} - c_j c_{j+r}) + \text{const}. \]  

(7)

Using the Majorana operators one can also write,

\[ H = \frac{i}{2} \sum_{r=-R}^{R} \sum_{j \in \Lambda} t_r \bar{\gamma}_j \gamma_{j+r}; \]  

(8)

where \( t_r = -(a_r + b_r) \) and \( t_{-r} = -(a_r - b_r) \). It is very useful to put the coupling constants as the coefficients of the following holomorphic function \( f(z) = \sum_r t_r z^r \). Then the Hamiltonian can be diagonalized by going to the Fourier space and then Bogoliubov transformation as follows, see for example\(^68\):

\[ H = \sum_q |f(q)| \eta_q \eta_q^\dagger + \text{const}, \]  

(9)
where \( \eta_q = \frac{1}{2} \left( 1 + \frac{f(q)}{|f(q)|} \right) c_{-q} + \frac{1}{2} \left( 1 - \frac{f(q)}{|f(q)|} \right) c_{-q} \) with \( f(q) := f(e^{i\theta}) \). Finally one can write the following explicit formula for the correlation matrix of the ground state:

\[
G_{jk} = \int_0^{2\pi} \frac{dq}{2\pi} \frac{f(q)}{|f(q)|} e^{iq(j-k)}.
\]

The above correlation matrix has a Toeplitz structure which makes it a suitable candidate for analytical calculations. It is possible to extend the above result to also excited states without much difficulty. When there is no translational invariance as it is the case for \( H_{\text{free}}(A',B') \) following the above procedure is not simple. An explicit calculations will be presented later for the transverse field XY chain with the staggered magnetization. In this work we will follow another path which is going to be one of our main results.

The basic idea of the second method is based on writing the Eq. (3) as the Eq. (6). We show here that there are others by proper manipulation of the rows and columns of the correlation matrix. For example, if \( G_{C} \) or \( F_{C} \) leads to the same set of FP’s as the \( C_{G} \) or \( C_{F} \) depends on the presence or the lack of a fermion at site \( j \). Now it is easy to show that we have

\[
\text{Min}[M] = \det \left( I - L_M \right) + I + I; \quad \text{Min}[M] = \det \left( I - L_M \right) M + I + I/2.
\]

where \( I \) is an identity matrix and \( L_M \) is a diagonal matrix made out of \( \pm 1 \) which clearly depends on which columns and rows are getting removed. We set its diagonal element to minus one when we have a fermion and one when there is no fermion at the corresponding site. Now it is easy to show that we have

\[
P(C) = \det \left( I - G_{C} \right)/2, \quad P(C) = \det \left( I - L_M G_{C} \right)/2.
\]

The above equations means that the formation probability \( P(C) \) is actually the EFP for a defect Hamiltonian with the correlation matrix \( GL_{C} \) or \( L_{C} G \). As we mentioned before none of these correlation matrices are necessarily the actual correlation matrix of the defect Hamiltonian \( H_{\text{free}}(A',B') \) introduced above. In fact we will show explicitly later that for the staggered Ising chain the correlation matrix has quite a different form. This should not be surprising because one can extract the minor of a matrix using quite different methods and although they all end up to the same number for \( P(C) \), they have been derived from different matrices. However, clearly finding one is enough to get the others by proper manipulation of the rows and columns of the correlation matrix. For example, if \( G' \) is the actual correlation matrix then there is a similarity transformation \( S \) which we have \( G' = S^{-1} C_{G} S \). For generic correlation matrices finding the \( S \) matrix is not necessarily an easy problem. It is worth mentioning that using the correlation matrices \( GL_{C} \) or \( L_{C} G \) leads to the same set of FP’s as the \( C \) matrix. In principle, the Eqs. (13) and (14) probably can be useful for analytical calculations when the \( C \) matrix is a Toeplitz matrix and the configuration \( C \) has a pattern. In these cases the \( GL_{C} \) has always a block Toeplitz structure. As an explicit example consider the ground state of the Hamiltonian (7) and let us focus on the probability of the configuration \( C = (s_1, s_2, ..., s_l) \), where \( s_j = -1 \) or \( +1 \) depending on the presence or the lack of a fermion at site \( j \). Then we can write:

\[
(G_{L})_{jk} = \text{sgn}_{\eta}(j,k) \int_0^{2\pi} \frac{dq}{2\pi} \frac{f(q)}{|f(q)|} e^{iq(j-k)},
\]

\[
(I_{C} G)_{jk} = \text{sgn}_{\ell}(j,k) \int_0^{2\pi} \frac{dq}{2\pi} \frac{f(q)}{|f(q)|} e^{iq(j-k)},
\]

where the matrices \( \text{sgn}_{\eta} \) and \( \text{sgn}_{\ell} \) are the sign matrices and for example for a configuration with four sites have the following forms:

\[
\text{sgn}_{\eta} = \begin{pmatrix}
  s_1 & s_1 & s_1 & s_1 \\
  s_2 & s_2 & s_2 & s_2 \\
  s_3 & s_3 & s_3 & s_3 \\
  s_4 & s_4 & s_4 & s_4
\end{pmatrix}, \quad \text{sgn}_{\ell} = \begin{pmatrix}
  s_1 & s_2 & s_3 & s_4 \\
  s_1 & s_2 & s_3 & s_4 \\
  s_1 & s_2 & s_3 & s_4 \\
  s_1 & s_2 & s_3 & s_4
\end{pmatrix}.
\]

The generalization for bigger sizes is straightforward. We note that when the configuration has a crystal structure the above matrices have block Toeplitz forms.
III. STATISTICS OF A GENERIC QUADRATIC OBSERVABLE AS A FORMATION PROBABILITY

In this section we argue that the problem of finding the statistics of a generic quadratic observable is essentially a FP problem and consequently the formulas derived in the previous section have much more applications than at first might appear. Consider the following quadratic observable

\[ O_D = c^\dagger Mc + \frac{1}{2} c^\dagger Nc^\dagger + \frac{1}{2} c^\dagger N^T c - \frac{1}{2} Tr M, \]  

(18)

where \( M \) and \( N \) are symmetric and anti-symmetric matrices respectively. It is much more convenient to write the above observable in the following form:

\[ O_D = \frac{1}{2} (c^\dagger, c) \begin{pmatrix} M & N \\ -N & -M \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}, \]  

(19)

Note that the above observable can have support just in a subsystem \( D \) of the full system. With the statistics of this observable we mean if the full system is in the ground state or any other state what is the probability of finding a particular value if we measure the above quantity. We prove here that this is a FP problem. To show this we first diagonalize the observable \( O_D \) with the standard method of Ref.\(^{67}\), see Appendix A. The idea is based on a canonical transformation

\[ \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = U \begin{pmatrix} \delta \\ \delta^\dagger \end{pmatrix}, \]  

(20)

which leads to

\[ O_D = \sum_k |\lambda_k| \delta_k^\dagger \delta_k - \frac{1}{2}. \]  

(21)

The eigenvalues and the eigenvectors of the observable can be derived as usual by applying the modes on the ground state properties. The next step is to write the Hamiltonian with respect to the \( \delta_k^\dagger \) and \( \delta_k \) as follows:

\[ \mathcal{H}_{\text{free}}(A, B) = \frac{1}{2} (\delta^\dagger, \delta) U \begin{pmatrix} A & B \\ -B & -A \end{pmatrix} U^\dagger \begin{pmatrix} \delta \\ \delta^\dagger \end{pmatrix}, \]  

(22)

The above equation can now be used to make the main argument. In the new basis if one calculates the FP with the new matrices the result is exactly equal to the probability of finding a particular value for the corresponding observable. For example, the EFP for the above Hamiltonian is exactly equal to the probability of finding the minimum value for the corresponding observable \( O_D \). To find the exact formula one first needs to calculate the correlation matrix

\[ iG'_{jk} = \langle \overline{\alpha}_j \alpha_k \rangle, \]  

(23)

where we defined the new Majorana operators \( \alpha_k = \delta_k + \delta_k^\dagger \) and \( \overline{\alpha}_j = i(\delta_j^\dagger - \delta_j) \). Having found the above correlation matrix the rest of the calculation is exactly as described in the previous section.

When the observable is defined for a subsystem one can also use the procedure that was outlined in \(^{28}\) which is based on the reduced density matrix. When the system is in the ground state the reduced density matrix can be written as:

\[ \rho_D = \det \frac{1}{2} (1 - G) e^{\mathcal{H}}, \]  

(24)

\[ \mathcal{H} = \frac{1}{2} (c^\dagger, c) \begin{pmatrix} M & N \\ -N & -M \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} + \frac{1}{2} Tr \ln (F_s), \]  

(25)

where \( \mathcal{H} \) is the entanglement Hamiltonian and

\[ \begin{pmatrix} M & N \\ -N & -M \end{pmatrix} = \ln \begin{pmatrix} F_s - F_a F_s^{-1} F_a \\ -F_s^{-1} F_a - F_a F_s^{-1} \end{pmatrix}, \]  

(26)

where \( F_a = F - F_s^T \) and \( F_s = F + F_s^T \) and as before \( F = \frac{1}{2} (1 + G) \). Note that the \( G \) matrix here is calculated for the original creation and annihilation operators appearing in the Hamiltonian. The idea is again based on writing the entanglement Hamiltonian in the basis in which the observable is diagonal, i. e. \( \delta \) basis. Now, we introduce the fermionic coherent states, i. e. \( |\gamma\rangle = |\gamma_1, \gamma_2, ..., \gamma_{|D|}\rangle = e^{-\sum_{k=1}^{|D|} \gamma_k \delta_k^\dagger} |0\rangle \), where \( \gamma_k \)’s are Grassmann numbers with the following
where we defined

\[ \bar{\mathbf{F}}_s = e^\mathbf{Y}, \quad \bar{\mathbf{F}} = \bar{X} + e^\mathbf{Y}, \]  

with

\[ \bar{X} = \hat{T}_{12}(\hat{T}_{22})^{-1}, \quad \bar{Z} = (\hat{T}_{22}^{-1})\hat{T}_{21}, \quad e^{-\mathbf{Y}} = \hat{T}_{22}^T, \]  

where

\[ \mathbf{T} = \begin{pmatrix} \hat{T}_{11} & \hat{T}_{12} \\ \hat{T}_{21} & \hat{T}_{22} \end{pmatrix} = \mathbf{U} \begin{pmatrix} \mathbf{F}_s - \mathbf{F}_s^{-1}\mathbf{F}_a\mathbf{F}_s^{-1} & \mathbf{F}_a\mathbf{F}_s^{-1} \\ -\mathbf{F}_s^{-1}\mathbf{F}_a & \mathbf{F}_s^{-1} \end{pmatrix} \mathbf{U}^\dagger. \]  

The equation (27) can be used to calculate all the desired probabilities using the same method that was developed in Ref.1. First of all, it is easy to see that to find the probability of finding the observable in its minimum value, one needs to put all the \( \gamma \)'s equal to zero, then we have

\[ p(o_{\text{min}}) = \det \frac{1}{2}(1 - \mathbf{G}) \left[ \frac{\det(\mathbf{F}_s)}{\det(\mathbf{F}_s^a)} \right]^\frac{1}{2}. \]  

To find the probability of other values, say \( o \), one needs to know the corresponding modes \( \lambda_k \)'s in which generate the desired eigenvalue of the observable and then, perform a Grassmann integral over the corresponding \( \gamma_k \)'s and put the other \( \gamma \)'s equal to zero. The result is

\[ p(o) = \det \frac{1}{2}(1 - \mathbf{G}) \left[ \frac{\det(\mathbf{F}_s)}{\det(\mathbf{F}_s^a)} \right]^\frac{1}{2} \sum_g \text{Min} \left[ \bar{\mathbf{F}} \right], \]  

where \( \text{Min} \left[ \bar{\mathbf{F}} \right] \) is the corresponding principal minor of the matrix \( \bar{\mathbf{F}} \) and the sum takes care of the degeneracies. Note that one can again use the equation (11) to get rid of the minor in the above equation. The above equation is very convenient to get explicit results for the probabilities without going through the generating function formalism.

**A. Statistics of the number of particles**

Statistics of the number of particles in a subsystem is the simplest possible example one can imagine because the observable itself is already diagonal. For earlier detailed studies regarding fluctuations of the particles from the generating function point of view see Refs.52–54. It is simple to see that the probability of finding no particle in the subsystem of size \( l \) is exactly the EFP. Then the probability of finding one particle is just about summing over all the FP’s with just one fermion. In other words we need to first calculate the sum of the minors of rank one of the matrix \( \mathbf{F} \). For generic case we need to find the sum of the minors of a particular rank of the matrix. There is a standard method to calculate these numbers which is called Faddeev-LeVerrier algorithm (see Wikipedia). The probability of having \( k \) particles can be explicitly written as:

\[ P(k) = \det \left[ \frac{1}{2}(1 - \mathbf{G}) \right] (-1)^k c_{l-k}, \]  

where the exact form of the coefficients can be written as:

\[ c_{l-k} = (-1)^{l-k} \frac{1}{k!} B_k(\text{tr} \mathbf{F}, -\text{tr} \mathbf{F}^2, 2!\text{tr} \mathbf{F}^3, \ldots, (-1)^{k-1}(k-1)!\text{tr} \mathbf{F}^k), \]  

where \( B_k \) is the complete exponential Bell polynomial (see Wikipedia). The complete exponential Bell polynomial can be written as:

\[ B_n(x_1, x_2, \ldots, x_{n-k+1}) = \sum_{k=1}^{n} B_{n,k}(x_1, x_2, \ldots, x_{n-k+1}), \]
where the partial exponential Bell polynomial $B_{n,k}$ is given by the equation.

$$B_{n,k}(x_1, x_2, \ldots, x_{n-k+1}) = \sum_{j_1, j_2, \ldots, j_{n-k+1}} \frac{n!}{j_1! j_2! \ldots j_{n-k+1}!} \left( \frac{x_1}{2!} \right)^{j_1} \left( \frac{x_2}{2!} \right)^{j_2} \cdots \left( \frac{x_{n-k+1}}{2!} \right)^{j_{n-k+1}},$$

(36)

where the sum is over all the non-negative $j_1, j_2, \ldots, j_{n-k+1}$ in a way that we have $j_1 + j_2 + \cdots + j_{n-k+1} = k$ and $j_1 + 2j_2 + \cdots + (n-k+1)j_{n-k+1} = n$.

The first few terms of the coefficients can be written as:

$$c_i = 1,$$

(37)

$$c_{i-1} = -\text{tr} F,$$

(38)

$$c_{i-2} = \frac{1}{2!}(\text{tr} F)^2 - \text{tr} F^2,$$

(39)

$$c_{i-3} = -\frac{1}{3!}(\text{tr} F)^3 - 3\text{tr} F^2 \text{tr} F + 2\text{tr} F^3).$$

(40)

Note that we also have $c_0 = (-1)^i \text{det} F$. It is worth mentioning that using the properties of the Bell’s polynomial one can also write the following recursion relation for the probabilities:

$$P(k) = -\frac{1}{k} \sum_{j=1}^{k} (-1)^j \text{tr} F^j P(k-j).$$

(41)

The above formulas indicate that the problem of finding statistics of the number of particles boils down to the calculation of the trace of different powers of the matrix $F$.

**B. Statistics of the kinks**

In this section we provide an example to show how the formalism of this section should be applied for a non-trivial observable. We would like to study the statistics of the following quantity:

$$K = \frac{l - 1}{2} + \frac{1}{2} \sum_{j=1}^{l-1} (c_j^+ - c_j)(c_{j+1}^+ + c_{j+1})$$

(42)

The reason that we call this quantity kink statistics comes from the spin representation of this quantity after Jordan-Wigner transformation, i.e. $c_j^+ = \prod_{i=1}^{j-1} \sigma_i^+ \sigma_j^-$, which leads to $K = \frac{l}{2} \sum_{j=1}^{l-1} (1 - \sigma_j^z \sigma_{j+1}^z)$. In this example we have:

$$M_{ij} = \frac{1}{2} \delta_{i,j+1} + \frac{1}{2} \delta_{i+1,j} \quad N_{ij} = \frac{1}{2} \delta_{i+1,j} - \frac{1}{2} \delta_{i,j+1}$$

(43)

Using the method of Appendix A one can diagonalize $K$. The $C$ matrix is simply $C_{ij} = \delta_{ij} - \delta_{i,1} \delta_{1,j}$, and its eigenvectors $\psi_{ij}(j) \equiv \psi_{ij}$ are chosen to be $\delta_{ij}$ (i being the label of the eigenvector). Showing the eigenvectors by $\kappa_i$, and using the Eq. A8 for $\kappa_i \neq 0$, we easily show that $\phi_{ij}(j) \equiv \phi_{ij} = \delta_{i,j+1}$. Using these eigenvectors the following forms for $g$ and $h$ can be obtained:

$$g_{i,j} = \frac{1}{2} \delta_{i,j} - \frac{1}{2} \delta_{i,j+1} + \frac{1}{2} \delta_{i,1} \delta_{j,l}$$

$$h_{i,j} = \frac{1}{2} \delta_{i,j} + \frac{1}{2} \delta_{i,j+1} - \frac{1}{2} \delta_{i,1} \delta_{j,l}$$

(44)

and the corresponding $U$ is:

$$U = \begin{pmatrix} g & h \\ h & g \end{pmatrix}. $$

(45)

The diagonal form of $K$ is then:

$$K = \sum_k \kappa(k) \eta_k^\dagger \eta_k$$

(46)
where

\[ \kappa(k) = \begin{cases} +1 & \text{if } 1 < k \leq l \\ 0 & \text{if } k = 1 \end{cases} \]

Having the \( U \) matrix now one can write the desired entanglement Hamiltonian in the basis of \( \eta \) and then use the equation (32) to calculate the probability of having particular number of kinks in the ground state of the quantum spin chain. We note that here we can have \( n = 0, 1, \ldots, l - 1 \) number of kinks with the degeneracies \( 2^{(l-1)n} \).

### C. Generating function and moments

In this section following the same lines of thinking as above we give new formulas regarding the generating function and moments of an arbitrary quadratic observables. Compared to the results in\(^6\) the new formulas have simpler forms. The generating function for an arbitrary operator \( O_D \) is defined as:

\[ M(z) = \text{tr} \left[ \rho_D e^{z O_D} \right]. \tag{48} \]

The trace can be calculated explicitly in the \( \delta \) representation and after some manipulations the final result is

\[ M(z) = \det \frac{1}{2} (I - G) \left[ \det(F_s) \right]^\frac{1}{2} \det \left[ I + e^{z \Lambda T} \right]^\frac{1}{2}; \tag{49} \]

where \( \Lambda = \left( \begin{array}{cc} |\lambda| & 0 \\ 0 & -|\lambda| \end{array} \right) \) is the matrix of the eigenvalues of the observable \( O_D \). After simple expansion we have

\[ M(z) = \det \left[ I + \sum_{n=1}^{\infty} \frac{z^n}{n!} \tilde{\tau}_n \right]^{\frac{1}{2}}; \tag{50} \]

where \( \tilde{\tau}_n = \Lambda^n \tilde{T} \). To calculate the moments we need to use the following formula\(^6\)

\[ \det \left[ I + \sum_{n=1}^{\infty} \frac{z^n}{n!} \tilde{\tau}_n \right] = 1 + \sum_{k=1}^{\infty} \frac{t_k}{k!}, \tag{52} \]

where

\[ t_k = \sum_{j=1}^{k} f_j B_{kj}(g); \tag{53} \]

and \( f_j = \frac{1}{2} \) and \( B_{kj}(g) \) is the partial exponential Bell polynomial defined as

\[ \frac{1}{j!} \left( \sum_{k=1}^{\infty} \frac{g_k e^k}{k!} \right)^j = \sum_{k=j}^{\infty} B_{kj}(g_1, \ldots, g_{k-j+1}) \frac{e^k}{k!}, \quad j = 0, 1, 2, \ldots, \tag{54} \]

where \( \epsilon \) is just a parameter. Here, we list the first few terms,

\[ t_0 = 1, \tag{55a} \]

\[ t_1 = f_1 g_1, \tag{55b} \]

\[ t_2 = f_1 g_2 + f_2 g_1^2, \tag{55c} \]

\[ t_3 = f_1 g_3 + f_2 (3g_1 g_2) + f_3 g_1^3, \tag{55d} \]

\[ t_4 = f_1 g_4 + f_2 (4g_1 g_3 + 3g_2^2) + f_3 (6g_1^2 g_2) + f_4 g_1^4, \tag{55e} \]

where \( g = (g_1, g_2, \ldots) \) with

\[ g_k = \sum_{j=1}^{k} (-1)^{j-1} (j-1)! \text{tr} B_{kj} (\tilde{T}), \tag{56} \]
where $\tilde{\tau} = (\tilde{\tau}_1, \tilde{\tau}_2, \ldots)$. The $\text{tr} B_{kj}(\tilde{\tau})$ can be calculated first by calculating $B_{kj}(g)$ and then symmetrization of all the terms $G_1 G_2 \ldots G_r \to \frac{1}{r!} \sum_r G_{\pi_1} G_{\pi_2} \ldots G_{\pi_r}$, where the $G_i$'s are any sequence of the $\{g_k\}$ and the sum is over all permutations. After having a symmetrized form for $B_{kj}(g)$, we can now replace $\{g_k\}$ with $\{\tilde{\tau}_k\}$ and derive the formulas for $\text{tr} B_{kj}(\tilde{\tau})$. Here, we list a few of the coefficients,

$$ g_1 = \text{tr} \tilde{\tau}_1, \quad \quad \quad (57a) $$

$$ g_2 = \text{tr} \left[ \tilde{\tau}_2 - \tilde{\tau}_1^2 \right], \quad \quad \quad (57b) $$

$$ g_3 = \text{tr} \left[ 3 \tilde{\tau}_3 - 3 \tilde{\tau}_1 \tilde{\tau}_2 + 2 \tilde{\tau}_1^3 \right], \quad \quad \quad (57c) $$

$$ g_4 = \text{tr} \left[ 4 \tilde{\tau}_4 - 4 \tilde{\tau}_1 \tilde{\tau}_3 - 3 \tilde{\tau}_2^2 + 12 \tilde{\tau}_1^2 \tilde{\tau}_2 - 6 \tilde{\tau}_1^4 \right], \quad \quad \quad (57d) $$

Finally we have

$$ E_m = \langle O^m_D \rangle = t_m. \quad \quad \quad (58) $$

The first two moments can be written as follows:

$$ E_1 = \frac{1}{2} \text{tr} \tilde{\tau}_1, \quad \quad \quad (59) $$

$$ E_2 = \frac{1}{2} \text{tr} \left[ \tilde{\tau}_2 - \tilde{\tau}_1^2 \right] + \frac{1}{4} \text{tr}^2 \tilde{\tau}_1 \quad \quad \quad (60) $$

It is also possible to get simple formulas for the fluctuations around the average:

$$ \tilde{E}_m = \langle (O_D - \langle O_D \rangle)^m \rangle. \quad \quad \quad (61) $$

The first few terms are:

$$ \tilde{E}_1 = 0, $$

$$ \tilde{E}_2 = \frac{g_2}{2}, $$

$$ \tilde{E}_3 = \frac{g_3}{2}, $$

$$ \tilde{E}_4 - 3 \tilde{E}_2^2 = \frac{g_4}{2}, $$

$$ \tilde{E}_5 - 10 \tilde{E}_2 \tilde{E}_3 = \frac{g_5}{2}. \quad \quad \quad (62) $$

The most general case can be written as,

$$ \sum_{j=1}^m (-1)^{j-1} (j-1)! B_{mj} (\tilde{E}_1, \tilde{E}_2, \ldots, \tilde{E}_{m-j+1}) = \frac{g_m}{2}. \quad \quad \quad (63) $$

Finally one can also write the cumulants defined as:

$$ \kappa_m = \frac{d^m}{dz^m} \log M(z)|_{z=0} \quad \quad \quad (64) $$

with respect to the $E_m$ and $\tilde{E}_m$ as follows(see Wikipedia):

$$ \kappa_m = \sum_{j=1}^m (-1)^{j-1} (j-1)! B_{mj} (0, \tilde{E}_2, \ldots, \tilde{E}_{m-j+1}), \quad \quad \quad (65) \quad \quad \quad \quad \quad \quad m > 0, $$

$$ \kappa_m = \sum_{j=1}^m (-1)^{j-1} (j-1)! B_{mj} (E_1, E_2, \ldots, E_{m-j+1}), \quad \quad \quad (66) \quad \quad \quad \quad \quad \quad m > 1. $$

The above formulas have relatively simpler form than the ones presented in\textsuperscript{62}. However, we note that here we assume that the observable should be first diagonalized and then the moments should be calculated. In the approach of\textsuperscript{62} no diagonalization is needed.
IV. TRANSVERSE FIELD XY CHAIN WITH A STAGGERED LINE DEFECT

In this section we would like to provide an exact determinant formula for the formation probability of the Neel sub-configuration, i.e. $|\uparrow\uparrow\downarrow\downarrow\cdots\rangle$, in the XY chain by a direct method, that is the configuration in which the spins are in the Neel state for the sites lying in the interval $[1,n]$. In principle the formulas (13) and (14) are explicit examples which lead to block Toeplitz matrices. However, the direct method has this advantage that one can get an exact formula for the correlation matrix of the line defect problem which can be useful for its own sake. In this section we first explicitly show that the FP of the Neel configuration is the EFP for the staggered XY Hamiltonian. Then we solve the line defect Hamiltonian by using the J-W transformation and find the exact correlation matrix and EFP for the ground state.

The Hamiltonian of the transverse field XY chain is:

$$H_{XY} = -J \sum_{l=1}^{L} \left( \frac{1 + \gamma}{4} \sigma_{l}^{x} \sigma_{l+1}^{x} + \frac{1 - \gamma}{4} \sigma_{l}^{y} \sigma_{l+1}^{y} \right) - \frac{\hbar}{2} \sum_{l=1}^{L} \sigma_{l}^{z},$$  \hspace{1cm} (67)

where $\sigma_{l}^{i}$ ($i = x, y, z$) are the Pauli matrices, $J$ is the exchange parameter and $\hbar$ is the magnetic field. The FP of the Neel state for the interval of length $n$ (which we take it always even) is readily found to be

$$P_{\uparrow \downarrow}(n) = \langle g | \left( \frac{1 - \sigma_{l}^{z}}{2} \right) \left( \frac{1 + \sigma_{l}^{z}}{2} \right) \cdots \left( \frac{1 + (-1)^{n-1} \sigma_{l}^{z}}{2} \right) | g \rangle = \langle g | \prod_{j=1}^{n} \frac{1 - \sigma_{l}^{z}}{2} | g' \rangle,$$  \hspace{1cm} (68)

where $| g \rangle$ is the ground state of the XY chain, $| g' \rangle = P_{\uparrow \downarrow}(n) | g \rangle$, and $P_{\uparrow \downarrow}(n)$ is the projection operator defined by $\prod_{j=1}^{2} \sigma_{2j}$, satisfying the relation $(P_{\uparrow \downarrow}(n))^{2} = 1$. One can easily check that $| g' \rangle$ is the ground state of $H'_{XY} = P_{\uparrow \downarrow}(n) H_{XY} P_{\uparrow \downarrow}(n)$ with the same ground state energy as $H_{XY}$. Therefore, $P_{\uparrow \downarrow}(n)$ is the EFP (represented by $P(n)$ defined as the probability that all spins are down) of the ground state of $H'_{XY}$. After applying $P_{\uparrow \downarrow}(n)$, we find that the explicit form of $H'_{XY}$ is:

$$H'_{XY} = -J \sum_{l=1}^{L} \left( \frac{1 + \gamma}{4} \sigma_{l}^{x} \sigma_{l+1}^{x} + \frac{1 - \gamma}{4} f_{n}(l) \sigma_{l}^{y} \sigma_{l+1}^{y} \right) - \frac{\hbar}{2} \sum_{l=1}^{L} h_{n}(l) \sigma_{l}^{z},$$  \hspace{1cm} (69)

where $f_{n}(l) = -1$ and $h_{n}(l) = (-1)^{l+1} \hbar$ for the case $l \leq n$, and $f_{n}(l) = +1$ and $h_{n}(l) = +\hbar$ for the case $l > n$. To work with fermionic Hamiltonian corresponding to the spin chain, we use J-W transformation defined by

$$c_{l}^{\dagger} = \prod_{j<l} \sigma_{j}^{x} \sigma_{j}^{+},$$
$$c_{l} = \prod_{j<l} \sigma_{j}^{x} \sigma_{j}^{-},$$  \hspace{1cm} (70)

where $\sigma_{l}^{+} = \frac{1}{2} (\sigma^{x} + i\sigma^{y})$, and $\sigma_{l}^{-} = \frac{1}{2} (\sigma^{x} - i\sigma^{y})$. The transformed Hamiltonian then becomes:

$$H'_{XY} = \frac{1}{2} \sum_{l=1}^{L} \left[ J_{n}(l) \left( c_{l}^{\dagger} c_{l+1} - c_{l} c_{l+1}^{\dagger} \right) + J_{\gamma}(l) \left( c_{l}^{\dagger} c_{l+1}^{\dagger} - c_{l} c_{l+1} \right) \right]$$
$$- \frac{NJ}{2} \left( c_{L}^{\dagger} c_{1} + \gamma c_{L}^{\dagger} c_{1} + H.C. \right) - \sum_{l=1}^{L} h_{n}(l) c_{l}^{\dagger} c_{l} + \frac{1}{2} \sum_{l=1}^{L} h_{n}(l),$$  \hspace{1cm} (71)

where

$$J_{n}(l) = \begin{cases} J & \text{if } l > n, \\
\gamma & \text{if } l \leq n. \end{cases} \quad \gamma_{n}(l) = \begin{cases} \gamma & \text{if } l > n, \\
1 & \text{if } l \leq n. \end{cases}$$  \hspace{1cm} (72)

Note that this Hamiltonian is identical to the free fermionic Hamiltonian corresponding to the XY model (without staggered interval) outside the staggered interval as expected. In the above equations $H.C.$ is the Hermitian conjugate terms and $N$ is the eigenvalue of $N = \prod_{j \leq L} (2c_{j}^{\dagger} c_{j} - 1)$ (note that $c_{L+1} = -Nc_{1}$). In the $\sigma^{z}$ basis, if the number of down spins is odd (or equivalently the odd number of fermionic vacancies), then $N \equiv -1$ (corresponding to the periodic boundary conditions in the fermionic representation, i.e. Ramond (R) sector), and in the other case (even
number of down spins) \( N \equiv +1 \) (corresponding to the antiperiodic boundary conditions, i.e. Neveu-Schwartz (NS) sector).

For the \( R \)-sector \( (N = -1) \) the fermionic Hamiltonian becomes periodic as follows (ignoring the constant term):

\[
H'_{XY} = \frac{1}{2} \sum_{l=1}^{L} \left[ J_n(l) \left( c_i^\dagger c_{i+1} - c_{i} c_{i+1}^\dagger \right) + J_\gamma(n)(l) \left( c_i^\dagger c_{i+1}^\dagger - c_{i} c_{i+1} \right) \right] \\
- \sum_{l=1}^{L} h_n(l)c_i^\dagger c_i + \frac{1}{2} \sum_{l=1}^{L} h_n(l),
\]

whereas for the \( N = +1 \) case, the periodicity is destroyed. To retrieve the periodicity, we can use the transformation \( \tilde{c}_i = \exp \left[ \frac{i\pi(N+1)}{2L} \right] c_i \), which results to \( \tilde{c}_{L+1} = \tilde{c}_1 \). The cost of this operation is that the allowed momentums become half-integer multiplications of \( \frac{2\pi}{L} \).

In the followings we denote the fermionic operators for both cases by \( c \) and \( c^\dagger \), keeping in mind that for the \( R \)-sector the momentums should be integer multiplications of \( \frac{2\pi}{L} \), whereas for the NS-sector they should be half-integers.

To proceed in finding the staggered spin probability, it is first useful to represent the same for the EFP for the ordinary transverse field \( XY \) chain which is well-studied in the literature\(^{11-12}\). It can be found using the equation (4). To make contact with the notation of \(^{11} \) it is useful to define the matrix \( S = \frac{i}{\pi} G^T \), where \( S_{ij}(n) = s_{ij}(1) + is_{ij}(2) \), \( s_{ij}(1) \equiv \langle c_i c_j \rangle \), and \( s_{ij}(2) \equiv i \langle c_i c_j \rangle \). Then the EFP of the \( XY \) model (i.e. with no staggered interval involved) is shown to be:

\[
P(n)|_{H_{XY}} = |\text{Det}(S(n))|.
\]

Additionally for this case, using the exact forms of the correlation functions one readily finds:

\[
S_{j,k}^{\text{free}}(n) = \frac{1}{2} \delta_{ij} + \int_0^{2\pi} \frac{dq}{2\pi} \frac{\sigma(q) e^{iq(j-k)}}{\sigma(q) e^{-iq(j-k)}},
\]

\[
\sigma(q) = \frac{1}{2} \left( \frac{\cos q - h - i\gamma \sin q}{\sqrt{(\cos q - h)^2 + \gamma^2 \sin^2 q}} \right),
\]

from which we see that

\[
G_{j,k} = -\int_0^{2\pi} \frac{dq}{2\pi} \sigma(q) e^{-iq(j-k)}.
\]

The matrix \( S(n) \) for the ordinary \( XY \) model is a Toeplitz matrix, for which the EFP as the determinant of \( S(n) \) can be found in the thermodynamic limit using the Fisher-Hartwig technique\(^{11} \). Also using the fact that \( a_1 = a_{-1} = \frac{1}{2} \), \( b_1 = \frac{1}{2} \), and \( a_0 = -h \) in Eq. (7), one readily finds

\[
f(q) \left| f(q) \right| = -\frac{J \cos q - h + i\gamma \sin q}{\Lambda(q)} = -\sigma(q)^*.
\]

which (noting that the \( G \) matrix is real) is compatible with the Eq. (10). For the present case (with the ground state \( |g'\rangle \)) we note that \( P_{\gamma}(n)|_{H_{XY}} = P(n)|_{H'_{XY}} \), and therefore one should find a way to diagonalize \( H'_{XY} \). To this end, we use the recipe due to Lieb et. al\(^{67} \), according to which, after writing the Hamiltonian in the form

\[
H'_{XY} = \sum_{i,j} \left[ c_i^\dagger A_{i,j} c_j + \frac{1}{2} \left( \gamma \left( c_i^\dagger B_{i,j} c_j^\dagger \right) + h.c. \right) \right],
\]

one finds the energy spectrum by diagonalizing \( C = (A - B)(A + B) \). The details of this calculation can be found in the Appendices (A) and (B). The matrix \( C \) for \( H'_{XY} \) has the following form:

\[
C_{ii} = \hbar^2 + \frac{1}{2} J^2 (1 + \gamma^2), \quad
C_{i,i+1} = \begin{cases} (-1)^{i+h}J & \text{if } i \leq n \\ -hJ & \text{if } i > n \end{cases} \quad
C_{i,i+2} = \begin{cases} -\frac{1}{4} J^2 (1 - \gamma^2) & \text{if } i \leq n \\ \frac{1}{4} J^2 (1 - \gamma^2) & \text{if } i > n \end{cases}
\]
also $C_{i,j} = -hJ$ if $i = 1, j = L$ or $i = L, j = 1$ and $C_{i,j} = 0$ for other cases. Following Ref.\textsuperscript{67} one can find the eigenvalues and the eigenvectors of $C$, the eigenvalues of which is represented by $\Lambda^2_i$, being the square of the energy spectrum of the system without the line defect, see Appendices (A) and (B) for details. Since $A$ ($B$) is symmetric (antisymmetric), $(A-B)/(A+B)$ and $(A+B)/(A-B)$ are symmetric and their eigenvalues are real and the eigenvectors $\psi$ and $\phi$ (see Eqs. (A10) and (A11)) can be chosen to be orthogonal. To find such solutions, we use the trial function:

$$\psi_{kj} = \left[\frac{1+(-1)^j}{2}\right] (a_1 \sin km_j + a_2 \cos km_j) + \left[\frac{1-(-1)^j}{2}\right] (a_3 \sin km_j + a_4 \cos km_j),$$

(79)

where $k$ labels the eigenfunctions, $j$ is the number of the sites in the real space, $m_j \equiv \left\lfloor \frac{j+1}{2} \right\rfloor$, and $a_1, a_2, a_3, a_4$ are the coefficients which have to be fixed using the Eq. (A10). This pairing mechanism facilitates the calculations (note that sin and cos are exact solutions for $m_j \gg m_0 \equiv \frac{2}{3}$, and $m_j \ll m_0$). The strategy is as follows: We find two kinds of solutions: one for deep inside the staggered interval (DISI), and the other for deep outside the staggered interval (DOSI) with different coefficients. Then we should glue them by fulfilling the requirements at $j = 1$ and $j = n$, i.e. where the staggered interval begins and ends respectively. This has been done in Appendix (B) by details. There we show that the solutions at DISI and DOSI are the same, up to a phase shift $k_s \rightarrow k_s - \pi$ where $k_s = \frac{2\pi}{L}s$ is the twice of the real momentum $q_s$ which is $q_s = \frac{2\pi}{L}s$ for $N = -1$ (R sector) and $q_s = \frac{2\pi}{L}(s + \frac{1}{2})$ for $N = +1$ (NS sector) and $s$ runs over $-\frac{L}{2}, -\frac{L}{2} + 1, \ldots, \frac{L}{2} - 1$. After applying the boundary conditions, one reach finally to the following function which diagonalizes $C$ (see Appendix (B)):

$$\psi_{sj} = \sqrt{\frac{2}{L}} \left\{ \begin{array}{l} (-1)^{m_j} \cos q_s [j - n] \cos q_s [j - n] \quad j \leq n \\ \cos q_s [j - n] \quad j > n \end{array} \right\},$$

(80)

with the eigenvalues $\Lambda^2_i = (J \cos q_s - h)^2 + \gamma^2 \sin^2 q_s$. The other independent solution is obtained by replacing cos by sin. We consider the above solution for $q_s \leq 0$, and the sin solution for $q_s > 0$. To continue we should find the other solution ($\phi_{sj}$) which can easily be obtained using Eq. (A9), for $\Lambda_q \neq 0$:

$$\phi_{XY} (j \leq n) = -\sqrt{\frac{2}{L}} \left[ (-1)^{m_j} \frac{1 + \gamma}{2} \right] \cos q_s (j - n),$$

$$\phi_{XY} (j = n + 1) = -\sqrt{\frac{2}{L}} \left[ (-1)^{m_j} \frac{1 + \gamma}{2} \right] \cos q_s (j - n),$$

$$\phi_{XY} (j > n + 1) = -\sqrt{\frac{2}{L}} \left[ (-1)^{m_j} \frac{1 + \gamma}{2} \right] \cos q_s (j - n) + \frac{1 + \gamma}{2} \cos q_s (j - n + 1),$$

(81)

where $a_j$ (not to be confused with the coefficients $a_1, a_2, a_3$ and $a_4$) is 1 if $j$ belongs to the first sublattice (odd $j$s) and 0 for the other sublattice (even $j$s). This solution is reserved for $s \leq 0$, and for $q_s > 0$ one should replace cos by sin. For $\Lambda_q = 0$ the solution is $\phi(j) = \pm \psi(j)$. Having $\psi$ and $\phi$ solutions in hand, one can directly calculate $g_{si} \equiv \frac{1}{2} \langle \psi_{si} + \phi_{si} \rangle$ and $h_{si} \equiv \frac{1}{2} \langle \psi_{si} - \phi_{si} \rangle$ to diagonalize $H$, see relation A4. For example $\langle c_i c_j \rangle = \sum_{s} g_{si} h_{sj}$ where $s$ is integer (half-integer) for $N = -1$ ($N = +1$). Working out with $f_{i,j}^{\psi \phi} = \sum_{s} g_{si} B_{sj}$, in which $A, B = \psi, \phi$, one can easily show that always (irrespective to the amount of $i$ and $j$ being inside or outside the staggered interval) $f_{i,j}^{\psi \psi} = f_{i,j}^{\phi \phi} = \delta_{ij}$, and $\delta_{ij}$ is the Kronecker delta. These functions help us to calculate the important correlation functions:

$$\langle c_i c_j \rangle = \frac{1}{4} \left[f_{i,j}^{\psi \psi} + f_{i,j}^{\phi \phi} + f_{i,j}^{\phi \psi} + f_{i,j}^{\psi \phi}\right],$$

$$\langle c_i^d c_j^d \rangle = \frac{1}{4} \left[f_{i,j}^{\psi \psi} - f_{i,j}^{\phi \phi} + f_{i,j}^{\phi \psi} - f_{i,j}^{\psi \phi}\right],$$

$$\langle c_i^d c_j \rangle = \frac{1}{4} \left[f_{i,j}^{\psi \psi} + f_{i,j}^{\phi \phi} - f_{i,j}^{\phi \psi} - f_{i,j}^{\psi \phi}\right],$$

$$\langle c_i^d c_j^d \rangle = \frac{1}{4} \left[f_{i,j}^{\psi \psi} - f_{i,j}^{\phi \phi} - f_{i,j}^{\phi \psi} + f_{i,j}^{\psi \phi}\right],$$

(82)
We now calculate the correlation functions explicitly. In what follows, we consider the case in which $i, j \leq n$, and extension to the other cases is straightforward. To calculate the correlation functions, we need the following identity that has been proved in Appendix (C):

$$\frac{1}{4} (f_{\psi_0} \pm f_{\phi_0}) = \chi_{ij}^+ \sigma_1(i,j) + \chi_{ij}^- \sigma_2(i,j),$$

(83)

where $\chi_{ij}^+ = \left[ \frac{1+(-)^{i+j}}{2} \right] (-)^{m_{j+1} - n_i}$ and $\chi_{ij}^- = \left[ \frac{1-(-)^{i+j}}{2} \right] (-)^{m_{j+1} - n_i}$, and also

$$\sigma_1(j,k) = \frac{1}{2L} \sum_s \cos q_s (k-j) \left( \frac{-h + \cos q_s}{\Lambda_s} \right) = \frac{1}{2L} \sum_s \left( \frac{-h + \cos q_s}{\Lambda_s} \right) e^{-i q_s (k-j)},$$

$$\sigma_2(j,k) = \frac{1}{2L} \sum_s \sin q_s (k-j) \left( \frac{\gamma \sin q_s}{\Lambda_s} \right) = \frac{i}{2L} \sum_s \left( \frac{\gamma \sin q_s}{\Lambda_s} \right) e^{-i q_s (k-j)},$$

(84)

where we have used the symmetry considerations to add extra zero contributions, and for the summation, $s$ is integer for the $R$-sector, and half-integer for the NS-sector. Therefore, if $i$ and $j$ belong to the same sublattice then we have:

$$\Sigma_1(i,j) \equiv \frac{1}{4} (f_{\psi_0} + f_{\phi_0}) = (-)^{m_{j+1} - n_i} \sigma_1(j-i),$$

$$\Sigma_2(i,j) \equiv \frac{1}{4} (f_{\psi_0} - f_{\phi_0}) = (-)^{m_{j+1} - n_i} \sigma_2(j-i),$$

(85)

and

$$\Sigma_1(i,j) = (-)^{m_{j+1} - n_i} \sigma_2(j-i),$$

$$\Sigma_2(i,j) = (-)^{m_{j+1} - n_i} \sigma_1(j-i),$$

(86)

if they belong to the different sublattices. Therefore, at this stage we can find the explicit form of the correlation functions, which are

$$\langle c_i c_j^\dagger \rangle = \frac{1}{2} \delta_{ij} + \chi_{ij}^+ \sigma_1(i,j) + \chi_{ij}^- \sigma_2(i,j),$$

$$\langle c_i c_j \rangle = \chi_{ij}^+ \sigma_2(i,j) + \chi_{ij}^- \sigma_1(i,j).$$

(87)

Also note that $\langle c_i c_j^\dagger \rangle = - \langle c_j c_i \rangle$ and $\langle c_i c_j \rangle = \delta_{ij} - \langle c_i c_j^\dagger \rangle$, that can be readily checked.

Finally we turn to the calculation of the formation probability of the Neel configuration which is the EFP for $H'_{XY}$. It can be determined by calculating $|\text{Det}(S_a)|$, the elements of which is $s_{ij} = \langle c_i c_j^\dagger \rangle - \langle c_i c_j \rangle$ as outlined above. Using the above correlation functions, one simply obtains:

$$s_{jk} = \frac{1}{2} \delta_{jk} + (\chi_{jk}^+ - \chi_{jk}^-) \sigma(j,k),$$

(88)

where

$$\sigma(j,k) \equiv \sigma_1(j,k) - \sigma_2(j,k) = \frac{1}{2L} \sum_{s=-L/2}^{L/2-1} \left( \frac{\cos q_s - h - i \gamma \sin q_s}{\Lambda_s} \right) e^{i q_s (j-k)}.$$

(89)

This matrix, in the $L \to \infty$ limit becomes

$$\sigma(j,k) = \frac{1}{2} \int \frac{dq}{2\pi} \sigma(q) e^{i q (j-k)},$$

(90)

where $\sigma(q)$ defined in the Eq. (75). $s_{jk}$ is compatible with the result for the free case, i.e. Eq. (75), except that here a sign matrix ($\text{sgn}(j,k) \equiv \chi_{jk}^+ - \chi_{jk}^-$) is multiplied. The closed form of this sign matrix is:

$$\text{sgn}(j,k) = \cos \pi (k-j) \left\{ \left( -(-)^{\frac{k+j}{2}} \left| \cos \frac{\pi}{2} (k-j) \right| + (-)^{\frac{k-j}{2}} \left| \sin \frac{\pi}{2} (k-j) \right| \right) \right\},$$

(91)
For example, the explicit form for the above sign matrix for \( n = 8 \) is

\[
\text{sgn} = \begin{bmatrix}
+ & + & - & - & + & - & - & + \\
+ & + & - & - & + & - & - & + \\
- & - & + & - & + & - & - & + \\
- & - & + & - & - & + & + & - \\
+ & + & - & - & + & + & - & - \\
+ & + & - & - & + & + & - & - \\
- & + & - & - & + & - & + & - \\
- & + & - & - & + & - & + & - \\
\end{bmatrix}
\]  \tag{92}

One can easily check that the above sign matrix is different from the ones suggested in (17). As we already discussed in section II there are different sign matrices that lead to the same FP’s but they come from different correlation matrices. It is worth mentioning that since the Hamiltonian of the transverse field XY chain that we considered here was with PBC we ended up to have R and NS sectors for the fermionic counterparts. Finding which one is the actual ground state of the spin system is a non-trivial problem. Since our line defect problem has the same eigenvalues the problem is similar to the clean case and we refer to\(^{70}\) for systematic study of the clean case. Note that the calculated sign matrix is not only correct for the ground state of R and NS sectors of the XY chain but also for the generic one dimensional translational invariant free fermions.

V. PROBABILITY DISTRIBUTION OF PARTICLE NUMBERS AND KINKS IN THE TRANSVERSE FIELD XY CHAIN

In this section we provide a couple of examples to show how the explicit formulas that we provided in the previous sections can be applied to calculate the probability distribution of quadratic observables. In both cases the model that we take is the ground state of the transverse field XY chain which has a rich phase diagram with three critical lines at \( h = 1, \gamma \neq 0; h = -1, \gamma \neq 0 \) and \( \gamma = 0, -1 < h < 1 \). Here we concentrate mostly on the non-negative transverse field part of the phase diagram and study probability distribution of particle numbers and kinks in the transverse field XY chain.

A. Probability distribution of magnetization

The first example is the distribution of the magnetization in the \( \sigma^z \) direction in an interval of size \( l \). This is equivalent to the distribution of the number of particles that we have studied in the section IIIA. The generating function of this quantity in the thermodynamic limit has been already studied in\(^{60}\), however, it does not seem to be straightforward to do the inverse Laplace transform analytically or numerically in the most generic cases. Using the formulas of the section IIIB with appropriate \( G \) and \( F \) matrices we can easily calculate this distribution numerically for arbitrary parameters of the Hamiltonian. The results are depicted in the Figure 1 which show clear change of behavior when we cross the critical line \( h = 1 \). The emergent oscillations in the region \( h \geq 1 \) are similar to the ones that have already been seen in the study of the EFP in\(^{11}\) and attributed to the competition between the energy cost of flipping a spin (controlled by \( h \)) and the superconducting terms which create and destroy fermions in pairs (controlled by \( \gamma \)). Although not shown here, similar oscillations also appear in the region \( -1 \geq h \) with peaks shifted to the left part of the graph. Since on the line \( \gamma = 0 \) we have a \( U(1) \) symmetry the number of particles is fixed and consequently the distribution is just a Dirac delta function. For small \( h \) the effect of increasing \( \gamma \) is just broadening the distribution by increasing the variance.

B. Probability distribution of kinks

As a second example of our formalism we discuss the distribution of kinks in the ground state of the XY-chain. Using the method that was provided in the section IIIB, we calculated with exact numerical calculations the probability of having different number of kinks in the ground state and presented the results in the Figure 2. Similar to the particle number distribution here too we have clear change of behavior around the critical line. However, the oscillations are now appearing in the regions \( -1 \geq h \geq 1 \). This is not surprising because the \( \sigma_j^z \) and \( \sigma_j^x \sigma_{j+1}^x \) have dual behavior. In the case of the transverse field Ising chain this duality is exact and it is called Kramers-Wannier(KW) duality which
FIG. 1. Probability distribution of the magnetization in the $\sigma^z$ direction in terms of $\gamma$ and $h$ for the XY-chain with $L = 200$ and $l = 30$.

FIG. 2. Probability distribution of the kinks in the $\sigma^x$ direction for the XY-chain ($L = 200$ and $l = 18$) using the exact diagonalization outlined in SEC III. The graph shows the dependence on $\gamma$ and $h$.

connects the Hamiltonian with the magnetic field $h$ to the one with the magnetic field $\tilde{h} \equiv \frac{1}{h}$. To see the effect of this duality on the distribution we plotted in the Figure 3 the particle number and kink distribution for two different dual magnetic fields. To make the comparison easy we mirrored and shifted (by one unit) one of the distributions. The two distributions are perfectly matching which is a nice way to see the effect of the KW duality on the FCS.

VI. CONCLUSIONS

In this paper we studied formation probabilities and full counting statistics of the quadratic observables in the free fermions and the corresponding spin chains in the most generic possible way. We first showed that the problem of FP of the ground state of a generic free fermion can be translated into an emptiness formation probability of a free fermionic Hamiltonian with defects. In one dimension the defect is a line but in higher dimensions it can have different forms. Using the same line of thinking we then provided new determinant formulas for the FP’s with respect to the correlation matrix of the ground state of the Hamiltonian. In the second part of the paper we studied FCS of a generic quadratic observable in the ground state of a generic free fermion Hamiltonian. We showed that the probability of finding a particular value for the observable is exactly a FP problem for a Hamiltonian written in the basis that diagonalizes the observable. We showed how this can be done for a full system and also for the subsystem in the most generic case. Two simple cases, i.e. fluctuations of particles and kinks were discussed to show how one
should implement the presented ideas. Finally, in the last section we solved the problem of the transverse field XY chain with an staggered magnetic line defect. We found exact correlation functions in and outside of the staggered region and provided a determinant formula for the FP of the staggered configuration in the ground state of the XY chain. Throughout the paper we tried to keep the discussion as general as possible except when we were presenting explicit examples to show how the procedure can be followed. Clearly one can take a particular model such as the XY chain and apply the presented methods. The numerical method to calculate these quantities are quite simple, however, to further push the analytical calculations in specific cases one normally needs to hire such methods as the generalized Fisher-Hartwig theorem which is beyond the scope of this paper and we hope to come back to them in future works.

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**Appendix A: Diagonalization of the Free Fermions**

In this subsection, we summarize the result of Ref. 67. Consider a generic quadratic observable with real couplings

$$O = \sum_{ij} \left[ c_i^\dagger M_{ij} c_j + \frac{1}{2} c_i^\dagger N_{ij} c_j^\dagger + \frac{1}{2} c_i N_{ji} c_j - \frac{1}{2} \text{Tr} M \right], \tag{A1}$$

where $c_i^\dagger$ and $c_i$ are fermionic creation and annihilation operators, and $i$ and $j$ run over the interval $\{1, 2, ..., L\}$. The Hermitian observable requires $M$ and $N$ to be symmetric and antisymmetric matrices respectively. To diagonalize the operator we use the following canonical transformation

$$\begin{pmatrix} c \\ c^\dagger \end{pmatrix} = U^\dagger \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix}, \tag{A2}$$

with

$$U = \begin{pmatrix} g & h \\ h^* & g^* \end{pmatrix}. \tag{A3}$$

which results to where $g$ and $h$ are $L \times L$ matrices, and the diagonal form of $O$ is

$$O = \sum_k |\lambda_k| (\eta_k^\dagger \eta_k - \frac{1}{2}). \tag{A4}$$
By requiring that $[\eta_k, O] = |\lambda_k|\eta_k$, it is found that:
\[
\eta_k g_{ki} = \sum_j (g_{kj} M_{ji} - h_{kj} N_{ji}) \\
\eta_k h_{ki} = \sum_j (g_{kj} N_{ji} - h_{kj} M_{ji})
\] (A5)
By defining new matrices $\psi$ and $\phi$ as follows
\[
g = \frac{1}{2} (\psi + \phi), \\
h = \frac{1}{2} (\psi - \phi)
\] (A6) (A7)
then Eq. A5 results to
\[
\Psi_k(M - N) = |\lambda_k|\Phi_k
\] (A8)
\[
\Phi_k(M + N) = |\lambda_k|^2 \Psi_k
\] (A9)
or equivalently
\[
\Psi_k(M - N)(M + N) = |\lambda_k|^2 \Psi_k
\] (A10)
\[
\Phi_k(M + N)(M - N) = |\lambda_k|^2 \Phi_k
\] (A11)
where $(\Phi_k)_i = \phi_{ki}$, and $(\Psi_k)_i = \psi_{ki}$. Therefore $\Psi_k$ and $\lambda_k$ can be calculated by solving the eigenvalue equation (A10), and for $\lambda_k \neq 0$, $\Phi_k$ can be determined using (A8). For $\lambda_k = 0$, one should solve Eq. A9 directly to obtain $\Phi_k$.

Having obtained $h$ and $g$, one can calculate the correlation matrix $G$ for the full system defined as
\[
G_{ij} = ((c_i^\dagger - c_i)(c_j^\dagger + c_j))
\] (A12)
In terms of $h$ and $g$, $G$ can be also calculated as follows:
\[
G = (h^\dagger - g^\dagger)(g + h)
\] (A13)
In the following sections we use the above construction to diagonalize the $XY$ Hamiltonian.

**Appendix B: Diagonalization of the staggered $XY$ model**

In this section we present the details of diagonalization of the (modified) $XY$ Hamiltonian. The observable of interest here is the formation probability of the staggered pattern. The general scheme is to apply a projection transformation in such a way that this probability becomes an EFP in a modified $XY$ Hamiltonian.

The formation probability for the staggered configuration $|\downarrow\uparrow\downarrow\uparrow\cdots\rangle$ at zero temperature is:
\[
P_{\text{stag}}(n) = \langle 0 \left| \left( \frac{1 - \sigma_1^z}{2} \right)^n \left( \frac{1 + \sigma_2^z}{2} \right)^n \cdots \left( \frac{1 + (-1)^n \sigma_z}{2} \right) \right| 0 \rangle
\]
\[
= \langle 0 \left| \prod_{j=1}^{\int(\frac{n}{2})} \sigma_2^z \left( \frac{1 - \sigma_2^z}{2} \right)^n \left( \frac{1 - \sigma_n^z}{2} \right) \cdots \left( \frac{1 - \sigma_n^z}{2} \right)^n \left( \frac{1 + (-1)^n \sigma_z}{2} \right) \right| 0 \rangle
\] (B1)
To go to the Fermionic section, we use the Jordan-Wigner (J-W) transformation (Eq. 70). After applying $P_x = \prod_{j=1}^{\int(\frac{n}{2})} \sigma_2^z$, and also J-W transformation we obtain the Eq. 69, from which we obtain:
\[
H'_{XY} = \frac{1}{2} \sum_{l=1}^{L-1} \left[ J_n(l) \left( c_{i}^{\dagger} c_{l+1} - c_{l}^{\dagger} c_{i+1} \right) + J_n(l) \left( c_{l+1}^{\dagger} c_{i+1}^{\dagger} - c_{i} c_{l+1} \right) \right]
\]
\[
- \frac{N J}{2} \left( c_{L}^{\dagger} c_{1} + \gamma c_{L}^{\dagger} c_{1}^{\dagger} + H.C. \right)
\]
\[
- \sum_{l=1}^{L} h_n(l) c_{l}^{\dagger} c_{l} + \frac{1}{2} \sum_{l=1}^{L} h_n(l)
\] (B2)
where the constants were defined in Eq. 72. Also note that \( c_{L+1} = -Nc_1 \), from which we see that for \( N = -1 \) one obtains:

\[
H'_{XY} = \frac{1}{2} \sum_{i=1}^{L} \left[ J_n(l) \left( c_i^\dagger c_{i+1} - c_i c_{i+1}^\dagger \right) + J_\gamma l(l) \left( c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1} \right) \right] - \sum_{i=1}^{L} h_n(l)c_i^\dagger c_i + \frac{1}{2} \sum_{l=1}^{L} h_n(l)
\]

If we write the modified XY Hamiltonian in the following form:

\[
H'_{XY} = \sum_{i,j} \left[ c_i^\dagger A_{i,j} c_j + \frac{1}{2} \left( c_i^\dagger B_{i,j} c_j^\dagger + h.c. \right) \right]
\]

then we have:

\[
A_{ij}(i \leq n \text{ and } j \leq n) = \begin{cases} (-1)^i h & \text{if } i = j \\ \frac{1}{2} \gamma J & \text{if } i = j \pm 1 \end{cases}, \quad A_{ij}(i > n \text{ or } j > n) = \begin{cases} -h & \text{if } i = j \pm 1 \\ \frac{1}{2} J & \text{if } i = 1, j = L \text{ or } i = L, j = 1 \\ 0 & \text{otherwise} \end{cases}
\]

Also

\[
B_{ij}(i \leq n \text{ and } j \leq n) = \begin{cases} \frac{1}{2} J & \text{if } i = j + 1 \\ \frac{1}{2} J & \text{if } i = j - 1 \\ 0 & \text{otherwise} \end{cases}, \quad B_{ij}(i > n \text{ or } j > n) = \begin{cases} \frac{1}{2} \gamma J & \text{if } i = j + 1 \\ -\frac{1}{2} \gamma J & \text{if } i = j - 1 \\ 0 & \text{otherwise} \end{cases}
\]

Therefore one obtains the following form for \( C \equiv (A - B)(A + B) \):

\[
C_{ii} = h^2 + \frac{1}{2} J^2 (1 + \gamma^2)
\]

\[
C_{i,i+1} = \begin{cases} (-1)^i h J & \text{if } i \leq n \\ -h J & \text{if } i > n \end{cases}
\]

\[
C_{i,i+2} = \begin{cases} -\frac{1}{2} J^2 (1 - \gamma^2) & \text{if } i \leq n \\ \frac{1}{2} J^2 (1 - \gamma^2) & \text{if } i > n \end{cases}
\]

Note that \( C \) is symmetric, and also \( C_{L-1,1} = C_{L,2} = C_{1,L-1} = C_{2,L} = \frac{1}{2} J^2 (1 - \gamma^2) \), and also \( C_{i,L} = C_{L,i} = -hJ \). All other components of \( C \) are zero. We use the Eq. 79 to diagonalize this matrix and obtain \( \Lambda_k \)'s and also \( \Psi \). We analyze two cases separately: \( m \ll \frac{n}{2} \) (deep inside the staggered interval, or DISI region), and \( m \gg \frac{n}{2} \) (deep outside the staggered interval, or DOSI region).

**DISI case:**

For the solution, we consider the trial function Eq. 79 with constants \( a_1, a_2, a_3 \) and \( a_4 \) coefficients to be determined. This function can be re-written in the following form:

\[
\psi(m) = \begin{cases} a_1 \sin km + a_2 \cos km & \text{for the odd sublattice} \\ a_3 \sin km + a_4 \cos km & \text{for the even sublattice} \end{cases}
\]

In this case, applying Eq. A10, we end up with two set of equations (due to the bipartite nature of the lattice) to be solved (for DISI):

\[
(1) \quad \sin km \left( -\frac{1}{2} a_1 J^2 (1 - \gamma^2) \cos k + a_3 h J (\cos k - 1) + a_4 h J \sin k + a_1 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) \\
+ \cos km \left( -\frac{1}{2} a_2 J^2 (1 - \gamma^2) \cos k - a_3 h J \sin k + a_4 h J (\cos k - 1) + a_2 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) = 0
\]

\[
(2) \quad \sin km \left( -\frac{1}{2} a_3 J^2 (1 - \gamma^2) \cos k + a_1 h J (\cos k - 1) - a_2 h J \sin k + a_3 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) \\
+ \cos km \left( -\frac{1}{2} a_4 J^2 (1 - \gamma^2) \cos k + a_1 h J \sin k + a_2 h J (\cos k - 1) + a_4 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) = 0
\]
Each component (the coefficients of $\sin km$ and $\cos km$) should be separately set to zero. Therefore, we obtain:

\[
\begin{align*}
\begin{cases}
\alpha_1 \zeta_k + a_3 h J (\cos k - 1) + a_4 h J \sin k = 0 \\
\alpha_2 \zeta_k - a_3 h J \sin k + a_4 h J (\cos k - 1) = 0 \\
a_3 \zeta_k + a_1 h J (\cos k - 1) - a_2 h J \sin k = 0 \\
a_4 \zeta_k + a_1 h J \sin k + a_2 h J (\cos k - 1) = 0
\end{cases}
\end{align*}
\tag{B10}
\]

where $\zeta_k = -\frac{1}{2} J^2 (1 - \gamma^2) \cos k + h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2$. In the matrix form, we have:

\[
\begin{bmatrix}
\zeta_k & 0 & h J (\cos k - 1) & h J \sin k \\
0 & \zeta_k & -h J \sin k & h J (\cos k - 1) \\
h J (\cos k - 1) & -h J \sin k & \zeta_k & 0 \\
h J \sin k & h J (\cos k - 1) & 0 & \zeta_k
\end{bmatrix}
\begin{bmatrix}
a_1 \\
a_2 \\
a_3 \\
a_4
\end{bmatrix} = 0
\tag{B11}
\]

By setting the determinant to zero, we find that the eigenvalues should be of the following form:

\[
\Lambda_k^2 = \frac{1}{2} \left[ 2h^2 + J^2 (1 + \gamma^2) - J^2 (1 - \gamma^2) \cos k \pm 4 h J \sin^2 k \right]
\tag{B12}
\]

and the corresponding eigenvectors are:

\[
\eta^- = \begin{pmatrix} -\cos \frac{k}{2} \\ \sin \frac{k}{2} \\ 0 \\ 1 \end{pmatrix}, \quad \eta^+ = \begin{pmatrix} \sin \frac{k}{2} \\ \cos \frac{k}{2} \\ 0 \\ 1 \end{pmatrix}, \quad \eta_1^+ = \begin{pmatrix} \cos \frac{k}{2} \\ -\sin \frac{k}{2} \\ 0 \\ 1 \end{pmatrix}, \quad \eta_2^+ = \begin{pmatrix} -\sin \frac{k}{2} \\ \cos \frac{k}{2} \\ 0 \\ 1 \end{pmatrix}
\tag{B13}
\]

where the minus (plus) sign refers to minus (plus) sign in the eigenvalues.

**DOSI**

Now let us work out with DOSI following the same steps as the DISI case. Let us consider the coefficients to be $b_1$, $b_2$, $b_3$ and $b_4$. The equation governing $\Psi$ results to the following linear equations:

\[
\begin{cases}
(1) \quad \sin km \left( \frac{1}{2} b_1 J^2 (1 - \gamma^2) \cos k - b_3 h J (\cos k + 1) - b_4 h J \sin k + b_1 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) \\
+ \cos km \left( \frac{1}{2} b_2 J^2 (1 - \gamma^2) \cos k + b_3 h J \sin k - b_4 h J (\cos k + 1) + b_2 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) = 0 \\
(2) \quad \sin km \left( \frac{1}{2} b_3 J^2 (1 - \gamma^2) \cos k - b_1 h J (\cos k + 1) + b_2 h J \sin k + b_3 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) \\
+ \cos km \left( \frac{1}{2} b_4 J^2 (1 - \gamma^2) \cos k - b_1 h J \sin k - b_2 h J (\cos k + 1) + b_4 (h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2) \right) = 0
\end{cases}
\tag{B14}
\]

resulting to:

\[
\begin{cases}
b_1 \zeta_k - b_3 h J (\cos k + 1) - b_4 h J \sin k = 0 \\
b_2 \zeta_k + b_3 h J \sin k - b_4 h J (\cos k + 1) = 0 \\
b_3 \zeta_k + b_1 h J (\cos k + 1) + b_2 h J \sin k = 0 \\
b_4 \zeta_k - b_1 h J \sin k - b_2 h J (\cos k + 1) = 0
\end{cases}
\tag{B15}
\]

or, in the matrix form:

\[
\begin{bmatrix}
\zeta_k' & 0 & -h J (\cos k + 1) & -h J \sin k \\
0 & \zeta_k' & -h J \sin k & h J (\cos k + 1) \\
-h J (\cos k + 1) & h J \sin k & \zeta_k & 0 \\
-h J \sin k & -h J (\cos k + 1) & 0 & \zeta_k'
\end{bmatrix}
\begin{bmatrix}
b_1 \\
b_2 \\
b_3 \\
b_4
\end{bmatrix} = 0
\tag{B16}
\]

where $\zeta_k' = \frac{1}{2} J^2 (1 - \gamma^2) \cos k + h^2 + \frac{1}{2} J^2 (1 + \gamma^2) - \Lambda_k^2$. The corresponding eigenvalues are:

\[
\Lambda_k^2 = \frac{1}{2} \left[ 2h^2 + J^2 (1 + \gamma^2) + J^2 (1 - \gamma^2) \cos k \pm 4 h J \cos^2 k \right]
\tag{B17}
\]
This form is just like the eigenvalues found for the DISI, with different sign for \( J^2(1 - \gamma^2) \cos k \). The corresponding eigenvectors are:

\[
\eta^-_1 = \begin{pmatrix} \sin \frac{k}{2} \\ \cos \frac{k}{2} \end{pmatrix}, \quad \eta^-_2 = \begin{pmatrix} -\sin \frac{k}{2} \\ 1 \end{pmatrix}, \quad \eta^+_1 = \begin{pmatrix} -\cos \frac{k}{2} \\ 0 \end{pmatrix}, \quad \eta^+_2 = \begin{pmatrix} \cos \frac{k}{2} \\ 1 \end{pmatrix}
\] (B18)

where again the the minus (plus) sign refers to the minus (plus) sign in the eigenvalues. Since we pair the sites in the direct space, the size of the first Brillouin zone is doubled. If we use the natural change \( k = 2q \), then we obtain:

\[
A^2_q = \frac{1}{2} \left[ 2h^2 + J^2(1 + \gamma^2) + J^2(1 - \gamma^2) \cos 2q \pm 4hJ \cos q \right]
\]

\[
= (J \cos q \pm h)^2 + J^2 \gamma^2 \sin^2 q
\] (B19)

that is exactly the spectrum of the single particle energies of the Fermions.

Summarizing, for DOSI, (using the above \( \eta \)'s) the full eigenvector is readily calculated to be:

\[
\psi^-_1 = \begin{cases} \cos k(m - \frac{1}{2}) \\ \cos km \end{cases}, \quad \psi^-_2 = \begin{cases} \sin k(m - \frac{1}{2}) \\ \sin km \end{cases}, \quad \psi^+_1 = \begin{cases} -\cos k(m - \frac{1}{2}) \\ \cos km \end{cases}, \quad \psi^+_2 = \begin{cases} -\sin k(m - \frac{1}{2}) \\ \sin km \end{cases}
\] (B20)

whereas for DISI,

\[
\psi^-_1 = \begin{cases} -\sin k(m - \frac{1}{2}) \\ -\cos km \end{cases}, \quad \psi^-_2 = \begin{cases} \cos k(m - \frac{1}{2}) \\ \cos km \end{cases}, \quad \psi^+_1 = \begin{cases} \sin k(m - \frac{1}{2}) \\ \sin km \end{cases}, \quad \psi^+_2 = \begin{cases} -\cos k(m - \frac{1}{2}) \\ -\sin km \end{cases}
\] (B21)

Interestingly we see that the phase shift \( k \to \pi - k \) relates the eigenvalues in DISI to the eigenvalues in DOSI. Since we need that these eigenvalues be equal for the case of line defect, we should apply this phase shift for one of the regions, e.g. DISI. Under this action, \( \cos k(m - \frac{1}{2}) \to -(1)^m \sin k(m - \frac{1}{2}), \sin k(m - \frac{1}{2}) \to -(1)^m \cos k(m - \frac{1}{2}), \cos km \to (1)^m \cos km \) and \( \sin km \to -(1)^m \sin km \). Therefore, for the DISI:

\[
\psi^-_1 \to \begin{cases} -(1)^{m+1} \cos k(m - \frac{1}{2}) \\ (1)^m \cos km \end{cases} = (1)^m \times \begin{cases} \cos k(m - \frac{1}{2}) \\ (1)^m \cos km \end{cases}
\]

\[
\psi^-_2 \to \begin{cases} -(1)^{m+1} \sin k(m - \frac{1}{2}) \\ (1)^m \sin km \end{cases} = (1)^m \times \begin{cases} \sin k(m - \frac{1}{2}) \\ (1)^m \sin km \end{cases}
\]

\[
\psi^+_1 \to \begin{cases} -(1)^{m+1} \cos k(m - \frac{1}{2}) \\ (1)^m \cos km \end{cases} = (1)^m \times \begin{cases} -\cos k(m - \frac{1}{2}) \\ (1)^m \cos km \end{cases}
\]

\[
\psi^+_2 \to \begin{cases} -(1)^{m+1} \sin k(m - \frac{1}{2}) \\ (1)^m \sin km \end{cases} = (1)^m \times \begin{cases} \sin k(m - \frac{1}{2}) \\ -\sin km \end{cases}
\] (B22)

showing that \( \psi_{DISI} = (1)^m \psi_{DOSI} \).

Now let us consider the chain as a whole, for which the boundary conditions at \( j = n \) should be worked out. To this end, we mix the two solutions obtained above. Based on the above findings, the following trial function is considered \( (m_0 = \lfloor \frac{n}{2} \rfloor) \):

\[
\psi(m \leq m_0) = (1)^m \times \begin{cases} a \cos k(m - \frac{1}{2}) + b \sin k(m - \frac{1}{2}) \\ a \cos km + b \sin km \end{cases}
\]

\[
\psi(m > m_0) = x \begin{cases} c \cos k(m - \frac{1}{2}) + d \sin k(m - \frac{1}{2}) \\ c \cos km + d \sin km \end{cases}
\] (B23)

With undetermined constants \( a, b, c, \) and \( d, \) to be found by applying the boundary conditions. To facilitate this calculation let us consider \( \gamma = 1 \) (pure Ising model). We have seen that the solution for the Ising model is also valid
for generic $\gamma$. For $\gamma = 1$ we have four independent equations at the boundaries:

\[
\begin{align*}
(a \cos km_0 + b \sin km_0) & - (c \cos k(m_0 + 1) + d \sin k(m_0 + 1)) + 2 \cos \frac{k}{2}(c \cos k(m_0 + \frac{1}{2}) + d \sin k(m_0 + \frac{1}{2})) = 0 \\
- (c \cos k(m_0) + d \sin k(m_0)) + (a \cos k + b \sin k) + 2 \cos \frac{k}{2}(-a \cos \frac{k}{2} - b \sin \frac{k}{2}) &= 0 \\
a \cos \frac{k}{2} + b \sin \frac{k}{2} - (c \cos \frac{k}{2} - d \sin \frac{k}{2}) + 2 \cos \frac{k}{2}(c \cos \frac{kL}{2} + d \sin \frac{kL}{2}) = 0 \\
- (a \cos k(m_0 - \frac{1}{2}) + b \sin k(m_0 - \frac{1}{2})) + (c \cos k(m_0 + \frac{1}{2}) + d \sin k(m_0 + \frac{1}{2})) + 2 \cos \frac{k}{2}(a \cos km_0 + b \sin km_0) = 0
\end{align*}
\] (B24)

These equations can be written in the matrix form:

\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} & a_{14} \\
a_{21} & a_{22} & a_{23} & a_{24} \\
a_{31} & a_{32} & a_{33} & a_{34} \\
a_{41} & a_{42} & a_{43} & a_{44}
\end{bmatrix}
\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = 0
\] (B25)

with the elements:

\[
\begin{align*}
a_{11} &= \cos km_0 \\
a_{12} &= \sin km_0 \\
a_{13} &= - \cos k(m_0 + 1) + 2 \cos \frac{k}{2}\cos k(m_0 + \frac{1}{2}) = \cos km_0 \\
a_{14} &= - \sin k(m_0 + 1) + 2 \cos \frac{k}{2}\sin k(m_0 + \frac{1}{2}) = \sin km_0 \\
a_{21} &= \cos k - 2 \cos^2 \frac{k}{2} = -1 \\
a_{22} &= \sin k - 2 \cos \frac{k}{2}\sin \frac{k}{2} = 0 \\
a_{23} &= - \cos \frac{kL}{2} \\
a_{24} &= - \sin \frac{kL}{2} \\
a_{31} &= \cos \frac{k}{2} \\
a_{32} &= \sin \frac{k}{2} \\
a_{33} &= - \cos \frac{k(L-1)}{2} + 2 \cos \frac{k}{2}\cos \frac{kL}{2} = \cos \frac{k}{2}(L+1) \\
a_{34} &= - \sin \frac{k(L-1)}{2} + 2 \cos \frac{k}{2}\sin \frac{kL}{2} = \sin \frac{k}{2}(L+1) \\
a_{41} &= - \cos k(m_0 - \frac{1}{2}) + 2 \cos \frac{k}{2}\cos km_0 = \cos k(m_0 + \frac{1}{2}) \\
a_{42} &= - \sin k(m_0 - \frac{1}{2}) + 2 \cos \frac{k}{2}\sin km_0 = \sin k(m_0 + \frac{1}{2}) \\
a_{43} &= \cos k(m_0 + \frac{1}{2}) \\
a_{44} &= \sin k(m_0 + \frac{1}{2})
\end{align*}
\] (B26)

The determinant of this matrix is $-4 \sin^2 \frac{k}{2} \sin^2 \frac{kL}{2}$, whose zeros take place at $k_s = \frac{4 \pi s}{L}$ in accordance with the free case (the case with no staggered interval involved). This is expected since the single particle energy spectrum of the original XY model should not change under the action of the unitary transformation $P_x$. For $\sin k_s m_0 \neq 0$ the solution for $a, b, c$ and $d$ is:

\[
a = - \cot k_s m_0, \quad b = -1, \quad c = \cot (k_s m_0), \quad d = 1
\] (B27)
This results to

\[ \psi(m \leq m_0) = -(-)^m \psi_0 \times \begin{cases} \cos k_s [m - m_0 - \frac{1}{2}] \\ \cos k_s [m - m_0] \end{cases} \]  
\[ \psi(m > m_0) = \psi_0 \begin{cases} \cos k_s [m - m_0 - \frac{1}{2}] \\ \cos k_s [m - m_0] \end{cases} \]  

(\text{B28})

where \( \psi_0 \) is the normalization factor, which is shown to be \( \sqrt{\frac{2}{L}} \). In terms of \( j = 2m_j \) and \( q_s = \frac{k_s}{2} \) we find that:

\[ \psi(j) = \sqrt{\frac{2}{L}} \begin{cases} (-1)^{m_j} \cos q_s [j - n] & j \leq n \\ \cos q_s [j - n] & j > n \end{cases} \]  

(\text{B29})

Also the other choice for \( a, b, c \) and \( d \) is

\[ a = \tan k_s m_0, \quad b = -1, \quad c = -\tan k_s m_0, \quad d = 1 \]  

(\text{B30})

which is equivalent to \( \cos \leftrightarrow \sin \). Although the Eq. B29 was obtained for \( \gamma = 1 \), it is a general result for the staggered line defect, and is valid for generic \( \gamma \).

\section*{Appendix C: Correlation functions}

Here we present the details of calculation of the correlation functions. In the previous Appendix we showed that the eigenvector of the matrix \( C \) for the \( XY \) model in the general form is:

\[ \psi_{XY} = \sqrt{\frac{2}{L}} \begin{cases} (-1)^{m_j} \cos q_s (j - n) & j \leq n \\ \cos q_s (j - n) & j > n \end{cases} \]  

(\text{C1})

Therefore using the relation A9 we obtain the general form of \( \phi_{st} \) for \( \Lambda_k \neq 0 \) (generic \( \gamma \)):

\[ \phi_{XY}(j \leq n) = -\Lambda_k^{-1} \sqrt{\frac{2}{L}} \left[ (-1)^{m_j + s_j} h \cos q_s (j - n) \right. \]
\[ \left. + \frac{1 + \gamma}{2} (-1)^{m_j - 1} \cos q_s (j - n - 1) + \frac{1 + \gamma}{2} (-1)^{m_j + 1} \cos q_s (j - n + 1) \right] \]

\[ \phi_{XY}(j = n + 1) = -\Lambda_k^{-1} \sqrt{\frac{2}{L}} \left[ h \cos q_s (j - n) \right. \]
\[ \left. + \frac{1 + \gamma}{2} (-1)^{m_j - 1} \cos q_s (j - n - 1) - \frac{1 + \gamma}{2} \cos q_s (j - n + 1) \right] \]

(\text{C2})

\[ \phi_{XY}(j > n + 1) = -\Lambda_k^{-1} \sqrt{\frac{2}{L}} \left[ h \cos q_s (j - n) \right. \]
\[ \left. + \frac{1 + \gamma}{2} \cos q_s (j - n - 1) - \frac{1 + \gamma}{2} \cos q_s (j - n + 1) \right] \]

We should \( \sin \leftrightarrow \cos \) as we go from positive \( q_s \)'s to negative ones.

Let us work with \( f_{i,j}^{AB} = \sum_{s=-\frac{L}{2}}^{L/2-1} A_{si} B_{sj} \), in which \( A, B = \psi, \phi \). The importance of these functions can be understood noting that:

\[ \langle c_i c_j \rangle = \frac{1}{4} \left[ f_{\psi \psi} + f_{\psi \phi} + f_{\phi \psi} + f_{\phi \phi} \right], \quad \langle c_i c_j \rangle = \frac{1}{4} \left[ f_{\psi \psi} - f_{\psi \phi} + f_{\phi \psi} - f_{\phi \phi} \right] \]

(\text{C3})

One can easily show that always (irrespective to the amount of \( i \) and \( j \) being inside or outside the staggered interval) \( f_{\psi \psi}^{i,j} = f_{\phi \phi}^{i,j} = \delta_{ij} \), and \( \delta_{ij} \) is the Kronecker delta. Having \( \Psi \) and \( \Phi \) in hand, one can directly calculate \( f_{\psi \psi}, f_{\phi \phi}, f_{\psi \phi}, \).
and $f_{\phi\psi}$. We immediately obtain that $f_{\psi\phi} = \delta_{ij}$ as expected. In the following we prove also that $f_{\phi\phi} = \delta_{ij}$. Let us consider $i \leq n$ and $j \leq n$. Then we have:

\[
\begin{align*}
\sum_{s} f_{\phi s} f_{s j} &= \frac{1}{L} \sum_{s} \left\{ (-)^{m_j + a_i - m_j - a_j} \frac{1}{2} (-)^{m_j - 1 - m_j - 1} \right\} \cos q_s (j - i) \\
&+ \frac{1}{L} \sum_{s} \left\{ (-)^{m_j + a_i - m_j - 1} \frac{1}{2} (-)^{m_j - 1 - m_j - 1} \right\} \cos q_s (j - i - 1) \\
&+ \frac{1}{L} \sum_{s} \left\{ (-)^{m_j + a_i - m_j - 1} \frac{1}{2} (-)^{m_j - 1 - m_j - 1} \right\} \cos q_s (j - i + 1) \\
&+ \frac{1}{L} \sum_{s} \left\{ (-)^{m_j + a_i - m_j - a_j} \frac{1}{2} (-)^{m_j - 1 - m_j - 1} \right\} \cos q_s (j - i - 2) \\
&+ \frac{1}{L} \sum_{s} \left\{ (-)^{m_j + a_i - m_j - a_j} \frac{1}{2} (-)^{m_j - 1 - m_j - 1} \right\} \cos q_s (j - i + 2) \\
&= (C4) \end{align*}
\]

Noting that $(-)^{m_i - 1} = (-)^{m_i + a_i} = (-)^{m_i + 1}$, we reach to:

\[
\begin{align*}
f_{\phi\phi} &= (-)^{m_j + 1 - m_i} \frac{1}{L} \sum_{s} \Lambda_s^{-2} \left( h^2 + \frac{1}{2} \left( 1 + \gamma^2 \right) \right) \cos q_s (j - i) \\
&+ (-)^{m_j + 1 - m_i - 1} \frac{1}{L} \sum_{s} \Lambda_s^{-2} \cos q_s (j - i - 1) \\
&+ (-)^{m_j + 1 - m_i - 1} \frac{1}{L} \sum_{s} \Lambda_s^{-2} \cos q_s (j - i + 1) \\
&= (C5)
\end{align*}
\]

leading to $\{ c_i^1, c_j \} = \frac{1}{2} (f_{\psi\phi} + f_{\phi\phi}) = \delta_{ij}$ as expected. Let us next calculate $f_{\psi\phi}$ and $f_{\phi\psi}$:

\[
\begin{align*}
f_{\psi\phi} &= (-)^{m_j + a_j - m_j - 1} \frac{1}{L} \sum_{s} \Lambda_s^{-1} \cos q_s (j - i) \\
&+ (-)^{m_j - 1 - m_i} \frac{1}{L} \sum_{s} \Lambda_s^{-1} \cos q_s (j - i - 1) \\
&+ (-)^{m_j + 1 - m_i} \frac{1}{L} \sum_{s} \Lambda_s^{-1} \cos q_s (j - i + 1) \\
&= (C6)
\end{align*}
\]
\[
f_{\phi\psi} = (-)^{m_i + a_i - m_j} h \frac{1}{L} \sum_s \Lambda_s^{-1} \cos q_s (j - i) \\
+ (-)^{m_i - 1 - m_j} \left( \frac{1 + \gamma}{2} \right) \frac{1}{L} \sum_s \Lambda_s^{-1} \cos q_s (j - i + 1) \\
+ (-)^{m_i + 1 - m_j} \left( \frac{1 + \gamma}{2} \right) \frac{1}{L} \sum_s \Lambda_s^{-1} \cos q_s (j - i - 1) \\
= (-)^{m_i + 1 - m_j} \frac{1}{L} \sum_s \Lambda_s^{-1} \left[ -h \cos q_s (j - i) + \left( \frac{1 - \gamma}{2} \right) \cos q_s (j - i + 1) + \left( \frac{1 + \gamma}{2} \right) \cos q_s (j - i - 1) \right] \\
= (-)^{m_i - m_j + a_i} \frac{1}{L} \sum_s \Lambda_s^{-1} \left[ h \cos q_s (j - i) - \cos q_s \cos q_s (j - i) - \gamma \sin q_s \sin q_s (j - i) \right] \\
= (-)^{m_i - m_j + a_j} \frac{1}{L} \sum_s \Lambda_s^{-1} (-)^{a_i - a_j} \left[ h \cos q_s (j - i) - \cos q_s \cos q_s (j - i) - \gamma \sin q_s \sin q_s (j - i) \right] \\
= (-)^{m_i + 1 - m_j} \frac{1}{L} \sum_s \Lambda_s^{-1} (-)^{a_i - a_j} \left[ -h \cos q_s (j - i) + \cos q_s \cos q_s (j - i) + \gamma \sin q_s \sin q_s (j - i) \right]
\]

Therefore

\[
\frac{1}{4} (f_{\phi\psi} \pm f_{\psi\phi}) = \frac{1}{2} (-)^{m_i + 1 + m_j} \frac{1}{L} \sum_s \Lambda_s^{-1} \left\{ \left[ \frac{1 + (-)^{a_i - a_j}}{2} \right] \left[ -h \cos q_s (j - i) + \cos q_s \cos q_s (j - i) \right] - \gamma \left[ \frac{1 + (-)^{a_i - a_j}}{2} \right] \sin q_s \sin q_s (j - i) \right\} \\
= \chi_{ij}^+ \sigma_1 (i, j) + \chi_{ij}^- \sigma_2 (i, j)
\]

where \( \chi_{ij}^+ = \left[ \frac{1 + (-)^{a_i - a_j}}{2} \right] \) \((-)^{m_i + 1 + m_j}\) and \( \chi_{ij}^- = \left[ \frac{1 - (-)^{a_i - a_j}}{2} \right] \) \((-)^{m_j + 1 - m_i}\), and also

\[
\sigma_1 (j, k) = \frac{1}{2L} \sum_{s = -L/2}^{L/2 - 1} \cos q_s (k - j) \left( \frac{-h + \cos q_s}{\Lambda_s} \right) = \frac{1}{2L} \sum_{s = -L/2}^{L/2 - 1} \left( \frac{-h + \cos q_s}{\Lambda_s} \right) e^{-iq_s (k - j)} \\
\sigma_2 (j, k) = \frac{1}{2L} \sum_{s = -L/2}^{L/2 - 1} \sin q_s (k - j) \left( \frac{\gamma \sin q_s}{\Lambda_s} \right) = \frac{i}{2L} \sum_{s = -L/2}^{L/2 - 1} \left( \frac{\gamma \sin q_s}{\Lambda_s} \right) e^{-iq_s (k - j)}
\]

where we have used the symmetry considerations to add extra zero contributions. Therefore if \( i \) and \( j \) belong to the same sublattice, then \( \chi_{ij}^+ = \left[ (-)^{m_j + 1 - m_i}\right] \) and \( \chi_{ij}^- = 0 \), so that:

\[
\Sigma_1 (i, j) \equiv \frac{1}{4} (f_{\phi\psi} + f_{\psi\phi}) = \left[ (-)^{m_j + 1 - m_i}\right] \sigma_1 (j - i), \\
\Sigma_2 (i, j) \equiv \frac{1}{4} (f_{\phi\psi} - f_{\psi\phi}) = \left[ (-)^{m_j + 1 - m_i}\right] \sigma_2 (j - i)
\]

Also if they belong to the different sublattices, then \( \chi_{ij}^- = \left[ (-)^{m_j + 1 - m_i}\right] \) and \( \chi_{ij}^+ = 0 \), and therefore we find that:

\[
\Sigma_1 (i, j) = \left[ (-)^{m_j + 1 - m_i}\right] \sigma_2 (j - i), \\
\Sigma_2 (i, j) = \left[ (-)^{m_j + 1 - m_i}\right] \sigma_1 (j - i)
\]
The correlation functions now can be determined explicitly. Using Eq. C3 we find:

\[
\langle c_{i}c_{j}^{\dagger}\rangle = \frac{1}{2}\delta_{ij} + \Sigma_{1}(i, j)
\]

\[
= \frac{1}{2}\delta_{ij} + \chi_{ij}^{+}\sigma_{1}(i, j) + \chi_{ij}^{-}\sigma_{2}(i, j)
\]

\[
\langle c_{i}c_{j}\rangle = \Sigma_{2}(i, j)
\]

\[
= \chi_{ij}^{+}\sigma_{2}(i, j) + \chi_{ij}^{-}\sigma_{1}(i, j)
\]

\[
\langle e_{i}^{+}c_{j}\rangle = -\chi_{ij}^{+}\sigma_{2}(i, j) - \chi_{ij}^{-}\sigma_{1}(i, j) = -\langle c_{i}c_{j}\rangle
\]

\[
\langle e_{i}^{+}c_{j}\rangle = \frac{1}{2}\delta_{ij} - \chi_{ij}^{+}\sigma_{1}(i, j) - \chi_{ij}^{-}\sigma_{2}(i, j) = \delta_{ij} - \langle c_{i}c_{j}\rangle
\]

(C12)

Therefore, noting that \( s_{ij} = \langle c_{i}c_{j}^{\dagger}\rangle - \langle c_{i}c_{j}\rangle \), we see:

\[
s_{ij} = \frac{1}{2}\delta_{ij} + (\chi_{ij}^{+} - \chi_{ij}^{-})\sigma(i, j)
\]

(C13)

where we have defined:

\[
\sigma(j, k) \equiv \sigma_{1}(j, k) - \sigma_{2}(j, k) = \frac{1}{2L} \sum_{s=-L/2}^{L/2-1} \left( \frac{\cos q_{s} - h - i\gamma\sin q_{s}}{\Lambda_{s}} \right) e^{iq_{s}(j-k)}
\]

(C14)

which, in the \( L \to \infty \) limit becomes

\[
\sigma(j, k) = \frac{1}{2} \int \frac{dq}{2\pi} \sigma(q) e^{iq(j-k)}
\]

\[
\sigma(q) = \frac{\cos q - h - i\gamma\sin q}{\Lambda_{q}}
\]

(C15)

Noting also that:

\[
(-)^{m_{j+1} - m_{i}} = \begin{cases} (-)^{\frac{i-j+1}{2}} & \text{if } i, j \in (\text{different sublattices}) \\ (-)^{\frac{i-j}{2}} & \text{if } i, j \in (\text{same sublattice}) \end{cases}
\]

(C16)

which results to:

\[
s_{ij} = \frac{1}{2}\delta_{ij} + \cos\pi(j-i) \left\{ (-)^{\frac{i-j+1}{2}} \sin\frac{\pi}{2}(j-i) + (\pi)^{\frac{i-j-1}{2}} \cos\frac{\pi}{2}(j-i) \right\} \sigma(j-i)
\]

(C17)

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